## => d his

(FILE 'HOME' ENTERED AT 10:48:29 ON 13 AUG 2010)

FILE 'REGISTRY' ENTERED AT 10:48:38 ON 13 AUG 2010 STRUCTURE UPLOADED L142 S L1 L299804 S 5-6-7/SZ L3 L4163779 S 6-6-7/SZ L5376419 S 6-7/SZ

L6 5308 S L1 SSS FUL

4055 S L6 AND CAPLUS/LC L7

FILE 'CAPLUS' ENTERED AT 10:56:20 ON 13 AUG 2010

1078 S L6 L8

L9 141434 S L3 OR L4 OR L5

FILE 'REGISTRY' ENTERED AT 11:00:52 ON 13 AUG 2010

L10 STRUCTURE UPLOADED

L11 5245 S L10 SUB=L6 FUL L12 63 S L6 NOT L11

FILE 'CAPLUS' ENTERED AT 11:02:31 ON 13 AUG 2010

L13 25 S L12

FILE 'REGISTRY' ENTERED AT 11:02:39 ON 13 AUG 2010 L14

38 S L12 AND CAPLUS/LC

L15 25 S L12 NOT L14

FILE 'CAPLUS' ENTERED AT 11:03:03 ON 13 AUG 2010

1059 S L11 L16

L17 10 S L9 AND L13 L18 4 S L16 AND L17 10 S L17 OR L18 L19

=> d 11

L1 HAS NO ANSWERS

L1 STR

G1 OH, X, SO2

G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

10/560,953

=> d 110 L10 HAS NO ANSWERS L10 STR

G1 OH,X,SO2 G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total

L19 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:1597089 CAPLUS

DOCUMENT NUMBER: 152:75085

TITLE: Preparation of pyrimidodiazepine derivatives for use

as PLK1 inhibitors

INVENTOR(S): Cai, Jianping; Chen, Shaoqing; Chu, Xin-Jie; Luk,

Kin-Chun Thomas; Mischke, Steven Gregory; Sun,

Hongmao; Wovkulich, Peter Michael

PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.

SOURCE: PCT Int. Appl., 305pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P <i>P</i>	PATENT NO.				KIND DATE			APPLICATION NO.					DATE				
WC	WO 2009153197			A1 20091223			WO 2009-EP57144				20090610						
	W:	ΑE,	AG,	AL,	AM,	ΑΟ,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,
		CA,	CH,	CL,	CN,	СО,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,
		ES,	FI,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,
		ΚE,	KG,	ΚM,	KN,	ΚP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,
		MD,	ME,	MG,	MK,	MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PE,
		PG,	PH,	PL,	PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	ST,	SV,
		SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	ZA,	ZM,	ZW
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HR,	HU,
		ΙE,	IS,	IT,	LT,	LU,	LV,	MC,	MK,	MT,	NL,	NO,	PL,	PT,	RO,	SE,	SI,
		SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,
		TD,	TG,	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,
		ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM						
US 20090318408 A1 20091224 US 2009-485108 20090616						616											
PRIORITY APPLN. INFO.: US 2008-73388P P 20080618																	
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT																	
OTHER SOURCE(S): MARPAT 152:75085																	

GΙ

AB Title compds. I [R1 = H, alkyl, cycloalkyl, phenoxyethyl, etc.; R2 = H, Me, or Et; each R3 independently = H, Cl, F, alkyl, etc.; R4 = OH, OMe, NH2, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as PLK1 inhibitors. Thus, e.g., II was prepared by protection of cyclopentylamine followed by alkylation with formaldehyde, alkylation with Et bromodifluoroacetate, deprotection, heteroarylation with 2,4-dichloro-5-nitropyrimidine, reduction, cyclization, and amination with 4-amino-3-methoxybenzoic acid. I were evaluated in PLK1 inhibition assays, e.g., II demonstrated an IC50 value of 1 to 50 nM.

ΙI

```
ΙT
     1062243-48-4P
                        1137867-66-3P
                                           1137867-67-4P
     1137869-89-6P
                        1137870-06-4P
                                           1137870-07-5P
     1137870-10-0P
                        1137870-11-1P
                                           1137870-13-3P
     1137870-14-4P
                        1201691-04-4P
                                           1201691-14-6P
     1201691-49-7P
                        1201691-61-3P
                                           1201691-62-4P
     1201691-69-1P
                        1201691-79-3P
                                           1201691-81-7P
     1201691-84-0P
                        1201692-12-7P
                                           1201692-19-4P
                                           1201692-37-6P
     1201692-25-2P
                        1201692-32-1P
     1201692-43-4P
                        1201692-49-0P
                                           1201692-62-7P
     1201692-70-7P
                        1201692-78-5P
                                           1201692-86-5P
     1201692-94-5P
                        1201692-97-8P
                                           1201693-04-0P
     1201693-11-9P
                        1201693-12-0P
                                           1201693-15-3P
     1201693-23-3P
                        1201693-29-9P
                                           1201693-35-7P
     1201693-41-5P
                        1201693-46-0P
```

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of pyrimidodiazepine derivs. for use as PLK1 inhibitors) 1062243-48-4 CAPLUS

Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX

RN

CN

10/560,953

NAME)

RN 1137867-66-3 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy- (CA INDEX NAME)

RN 1137867-67-4 CAPLUS

CN Benzoic acid, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1137869-89-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-

tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxybenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1137870-06-4 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluoro- (CA INDEX NAME)

RN 1137870-07-5 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN 1137870-10-0 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methyl- (CA INDEX NAME)

RN 1137870-11-1 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl- (CA INDEX NAME)

RN 1137870-13-3 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy- (CA INDEX NAME)

RN 1137870-14-4 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201691-04-4 CAPLUS

CN Benzoic acid, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-14-6 CAPLUS

CN Benzoic acid, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN 1201691-49-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-3-methoxy-, 1,1-dimethylethyl ester, (3R,4S)-rel-(CA INDEX NAME)

Relative stereochemistry.

RN 1201691-61-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201691-62-4 CAPLUS

CN Carbamic acid, N-[3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]propyl]-, 9H-fluoren-9-ylmethyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 1201691-69-1 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-, 1,1-dimethylethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-79-3 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 3-[[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201691-81-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]propyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201691-84-0 CAPLUS

CN Carbamic acid, N-[cis-4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Relative stereochemistry.

RN 1201692-12-7 CAPLUS

Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-CN pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

1201692-19-4 CAPLUS RN

Benzoic acid, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-CN oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN

1201692-25-2 CAPLUS
Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-CN propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN 1201692-32-1 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{O} & \mathsf{H} & \mathsf{CO}_2\mathsf{H} \\ \mathsf{F} & \mathsf{N} & \mathsf{NH} & \mathsf{OMe} \end{array}$$

RN 1201692-37-6 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201692-43-4 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201692-49-0 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy-, methyl ester (CA INDEX NAME)

RN 1201692-62-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methylbenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201692-70-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethylbenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201692-78-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-(trifluoromethyl)benzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201692-86-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxybenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201692-94-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluorobenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201692-97-8 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluoro- (CA INDEX NAME)

RN 1201693-04-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluorobenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-11-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-12-0 CAPLUS

CN Benzoic acid, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN 1201693-15-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]benzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-23-3 CAPLUS

CN Benzoic acid, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[2-(2-thienyl)ethyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

RN 1201693-29-9 CAPLUS

CN Benzoic acid, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenylethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} Me & & & \\ \hline N & & & \\ F & & N & \\ \hline N & & NH & \\ \hline CH_2-CH_2-Ph & & \\ \end{array}$$

RN 1201693-35-7 CAPLUS

CN Benzoic acid, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(3-phenylpropyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

RN 1201693-41-5 CAPLUS

CN Benzoic acid, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[(1R,2S)-2-phenylcyclopropyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-46-0 CAPLUS

CN Benzoic acid, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-(CA INDEX NAME)

ΙT	1062243-51-9P	1108195-27-2P	1137867-37-8P
	1137867-38-9P	1137867-40-3P	1137867-41-4P
	1137867-45-8P	1137867-57-2P	1137867-58-3P
	1137867-59-4P	1137867-60-7P	1137867-61-8P

1137867-62-9P	1137867-64-1P	1137867-65-2P
1137867-68-5P	1137867-71-0P	1137867-79-8P
1137867-88-9P	1137867-89-0P	1137867-92-5P
1137867-93-6P	1137867-99-2P	1137868-01-9P
1137868-03-1P	1137868-52-0P	1137868-93-9P
1137868-97-3P	1137868-98-4P	1137868-99-5P
1137869-00-1P	1137869-02-3P	1137869-03-4P
1137869-09-0P	1137869-11-4P	1137869-15-8P
1137869-16-9P	1137869-17-0P	1137869-18-1P
1137869-21-6P	1137869-22-7P	1137869-90-9P
1201691-05-5P	1201691-06-6P	1201691-07-7P
1201691-08-8P	1201691-09-9P	1201691-10-2P
1201691-11-3P	1201691-12-4P	1201691-13-5P
1201691-15-7P	1201691-16-8P	1201691-17-9P
1201691-19-1P	1201691-20-4P	1201691-21-5P
1201691-22-6P	1201691-23-7P	1201691-24-8P
1201691-25-9P	1201691-26-0P	1201691-27-1P
1201691-28-2P	1201691-29-3P	1201691-30-6P
1201691-31-7P	1201691-32-8P	1201691-33-9P
1201691-34-0P	1201691-35-1P	1201691-36-2P
1201691-37-3P	1201691-38-4P	1201691-39-5P
1201691-40-8P	1201691-41-9P	1201691-42-0P
1201691-43-1P	1201691-44-2P	1201691-45-3P
1201691-46-4P	1201691-47-5P	1201691-48-6P
1201691-50-0P	1201691-51-1P	1201691-52-2P
1201691-53-3P	1201691-54-4P	1201691-55-5P
1201691-56-6P	1201691-57-7P	1201691-58-8P
1201691-59-9P	1201691-60-2P	1201691-63-5P
1201691-64-6P	1201691-65-7P	1201691-66-8P
1201691-67-9P	1201691-68-0P	1201691-70-4P
1201691-71-5P	1201691-72-6P	1201691-73-7P
1201691-74-8P	1201691-75-9P	1201691-76-0P
1201691-77-1P	1201691-78-2P	1201691-80-6P
1201691-82-8P	1201691-83-9P	1201691-85-1P
1201691-86-2P	1201691-87-3P	1201691-88-4P
1201691-89-5P	1201691-90-8P	1201691-91-9P
1201691-92-0P	1201691-93-1P	1201691-94-2P
1201691-95-3P	1201691-96-4P	1201691-97-5P
1201691-98-6P	1201691-99-7P	1201692-00-3P
1201692-01-4P	1201692-02-5P	1201692-03-6P
1201692-04-7P	1201692-06-9P	1201692-07-0P
1201692-08-1P	1201692-09-2P	1201692-10-5P
1201692-11-6P	1201692-13-8P	1201692-14-9P
1201692-15-0P	1201692-16-1P	1201692-17-2P
1201692 <b>-</b> 18-3P	1201692-20-7P	1201692-21-8P
1201 <b>69</b> 2-22-9P	1201692-23-0P	1201692-24-1P
1201692-26-3P	1201692-27-4P	1201692-28-5P
1201692-29-6P	1201692-30-9P	1201692-31-0P
1201692-33-2P	1201692-34-3P	1201692-35-4P
1201692-36-5P	1201692-38-7P	1201692-39-8P
1201692-40-1P	1201692-41-2P	1201692-42-3P
1201692-44-5P	1201692-45-6P	1201692-46-7P
1201692-47-8P	1201692-48-9P	1201692-50-3P
1201692-51-4P	1201692-52-5P	1201692-53-6P
1201692-54-7P	1201692-55-8P	1201692-56-9P
1201692-57-0P	1201692-58-1P	1201692-59-2P
1201692-60-5P	1201692-61-6P	1201692-63-8P
1201002 00 01	1201072 01 01	1201072 00 01

RN

1201692-64-9P	1201692-65-0P	1201692-66-1P
1201692-67-2P	1201692-68-3P	1201692-69-4P
1201692-71-8P	1201692-72-9P	1201692-73-0P
1201692-74-1P	1201692-75-2P	1201692-76-3P
1201692-77-4P	1201692-79-6P	1201692-80-9P
1201692-81-0P	1201692-82-1P	1201692-83-2P
1201692-84-3P	1201692-85-4P	1201692-87-6P
1201692-88-7P	1201692-89-8P	1201692-90-1P
1201692-91-2P	1201692-92-3P	1201692-93-4P
1201692-95-6P	1201692-96-7P	1201692-98-9P
1201692-99-0P	1201693-00-6P	1201693-01-7P
1201693-02-8P	1201693-03-9P	1201693-05-1P
1201693-06-2P	1201693-07-3P	1201693-08-4P
1201693-09-5P	1201693-10-8P	1201693-13-1P
1201693-14-2P	1201693-16-4P	1201693-17-5P
1201693-18-6P	1201693-19-7P	1201693-20-0P
1201693-21-1P	1201693-22-2P	

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidodiazepine derivs. for use as PLK1 inhibitors) 1062243-51-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1108195-27-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(4-hydroxybutyl)-3-methoxy- (CA INDEX NAME)

RN 1137867-37-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-cyclopropyl-3-methoxy-(CA INDEX NAME)

RN 1137867-38-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-3-azetidinyl)- (CA INDEX NAME)

RN 1137867-40-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(4-methyl-1-piperazinyl)- (CA INDEX NAME)

RN 1137867-41-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-3-methoxy- (CA INDEX NAME)

RN 1137867-45-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-4-piperidinyl-(CA INDEX NAME)

RN 1137867-57-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluoro-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137867-58-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)-(CA INDEX NAME)

RN 1137867-59-4 CAPLUS

CN Benzamide, 3-chloro-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137867-60-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)-3-(trifluoromethoxy)- (CA INDEX NAME)

RN 1137867-61-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methyl-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137867-62-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137867-64-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137867-65-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1137867-68-5 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

## 10/560,953

RN 1137867-71-0 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-3-methoxy- (CA INDEX NAME)

RN 1137867-79-8 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[1-(2-hydroxyethyl)-4-piperidinyl]-3-methoxy- (CA INDEX NAME)

RN 1137867-88-9 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-methoxy- (CA INDEX NAME)

RN 1137867-89-0 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & & \\ \hline O & & & & & \\ \hline N & & & & & \\ \hline F & & & & & \\ \hline N & & & & & \\ \hline OMe & & & & \\ \hline \end{array}$$

RN 1137867-92-5 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1137867-93-6 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-methyl- (CA INDEX

NAME)

RN 1137867-99-2 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1137868-01-9 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-(methylsulfonyl)-4-piperidinyl]- (CA INDEX NAME)

RN 1137868-03-1 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-4-piperidinyl-(CA INDEX NAME)

RN 1137868-52-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137868-93-9 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1137868-97-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & MeO & C-NH-CH_2-CH_2-N \\ \hline F & N & NH-CH_2-CH_2-N \\ \end{array}$$

RN 1137868-98-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1137868-99-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O \\ \hline N \\ \hline N \\ \hline N \\ \hline N \\ \hline NH \\ \hline OMe \\ \end{array}$$

RN 1137869-00-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(2-hydroxyethyl)-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline N & NH \\ \hline O & C-NH-CH_2-CH_2-OH \\ \hline O & OMe \\ \hline \end{array}$$

RN 1137869-02-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

RN 1137869-03-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1137869-09-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-1-piperidinyl-(CA INDEX NAME)

RN 1137869-11-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1137869-15-8 CAPLUS

CN Benzamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 1137869-16-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-(1-methylethyl)-4-piperidinyl]- (CA INDEX NAME)

RN 1137869-17-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)- (CA INDEX NAME)

RN 1137869-18-1 CAPLUS

CN Benzamide, N-(1-acetyl-4-piperidinyl)-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1137869-21-6 CAPLUS

CN Benzamide, N-(3S)-1-azabicyclo[2.2.2]oct-3-yl-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 1137869-22-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-(2,2,2-trifluoroethyl)-4-piperidinyl]- (CA INDEX NAME)

RN 1137869-90-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy-N-4-piperidinyl- (CA INDEX NAME)

RN 1201691-05-5 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-06-6 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1201691-07-7 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201691-08-8 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-4-piperidinyl-(CA INDEX NAME)

RN 1201691-09-9 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-[[4-[(4-amino-1-piperidinyl)carbonyl]-2-methoxyphenyl]amino]-9cyclobutyl-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & NH_2 \\ \hline O & N & MeO & C & N \\ \hline F & N & NH & NH \\ \hline \end{array}$$

RN 1201691-10-2 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201691-11-3 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-12-4 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

Me O 
$$C-NH-(CH_2)_3-NMe_2$$
  $C-NH-(CH_2)_3-NMe_2$  O  $C-NH-(CH_2)_3-NMe_2$ 

RN 1201691-13-5 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-3-methoxy- (CA INDEX NAME)

RN 1201691-15-7 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1201691-16-8 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-methyl- (CA INDEX NAME)

RN 1201691-17-9 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-4-piperidinyl- (CA INDEX NAME)

RN 1201691-19-1 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-[[4-[(4-amino-1-piperidinyl)carbonyl]phenyl]amino]-9-cyclobutyl-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

RN 1201691-20-4 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)-(CA INDEX NAME)

RN 1201691-21-5 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(tetrahydro-2H-pyran-4-yl)-(CA INDEX NAME)

RN 1201691-22-6 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-(CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1201691-23-7 CAPLUS

CN Benzamide, 4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-(CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1201691-24-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methylethyl)- (CA INDEX NAME)

RN 1201691-25-9 CAPLUS

CN Benzamide, N-cyclohexyl-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-26-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(2-methoxyethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & C-NH-CH_2-CH_2-OMe \\ \hline F & N & OMe \\ \end{array}$$

RN 1201691-27-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(3-methoxypropyl)- (CA INDEX NAME)

RN 1201691-28-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 1201691-29-3 CAPLUS

CN Benzamide, N-(cyclohexylmethyl)-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-30-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(3-thienylmethyl)- (CA INDEX NAME)

RN 1201691-31-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(3-furanylmethyl)-3-methoxy- (CA INDEX NAME)

RN 1201691-32-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(phenylmethyl)-(CA INDEX NAME)

RN 1201691-33-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[[4-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 1201691-34-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-phenylethyl)- (CA INDEX NAME)

RN 1201691-35-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-phenyl- (CA INDEX NAME)

RN 1201691-36-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(2-ethoxyethyl)-3-methoxy- (CA INDEX NAME)

RN 1201691-37-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(3-hydroxypropyl)-3-methoxy- (CA INDEX NAME)

RN 1201691-38-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[(3,5-dichlorophenyl)methyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-39-5 CAPLUS

CN Benzamide, N-[2-(1,3-benzodioxol-5-yl)ethyl]-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-40-8 CAPLUS

CN Benzamide, N-[(1S,2R)-2-(aminocarbonyl)cyclopentyl]-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-41-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-[(1-methylethyl)amino]propyl]- (CA INDEX NAME)

RN 1201691-42-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(4-methyl-1-

piperazinyl)ethyl]- (CA INDEX NAME)

RN 1201691-43-1 CAPLUS

CN Benzamide, N-(2-aminoethyl)-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-44-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(1-piperazinyl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & MeO & C-NH-CH_2-CH_2-N \\ \hline \\ F & N & NH-CH_2-CH_2-N \\ \hline \end{array}$$

RN 1201691-45-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(1H-indol-3-yl)ethyl]-

3-methoxy- (CA INDEX NAME)

RN 1201691-46-4 CAPLUS

CN Benzamide, N-[3-(cyclohexylamino)propyl]-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-47-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-3-hydroxy-, phenylmethyl ester, (3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-48-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-3-methoxy-, phenylmethyl ester, (3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-50-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[(3R,4S)-3-methoxy-4-piperidinyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-51-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-4-methoxy-, phenylmethyl ester, (3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-52-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)-2,2-dimethylpropyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-53-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(1H-imidazol-1-yl)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-54-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-(4-pyridinyl)-4-piperidinyl]- (CA INDEX NAME)

RN 1201691-55-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-cyclopentyl-4-piperidinyl)-3-methoxy- (CA INDEX NAME)

RN 1201691-56-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(2,2,6,6-tetramethyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201691-57-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-cyclopropyl-4-piperidinyl)-3-methoxy- (CA INDEX NAME)

RN 1201691-58-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(cis-4-hydroxycyclohexyl)-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-59-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(trans-4-hydroxycyclohexyl)-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-60-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-, 9H-fluoren-9-ylmethyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 1201691-63-5 CAPLUS

CN Benzamide, N-(3-aminopropyl)-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-64-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[1-(2-fluoroethyl)-4-piperidinyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-65-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-[3-(methylsulfonyl)propyl]-4-piperidinyl]- (CA INDEX NAME)

RN 1201691-66-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(4-morpholinyl)propyl]- (CA INDEX NAME)

RN 1201691-67-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(1-pyrrolidinyl)propyl]- (CA INDEX NAME)

RN 1201691-68-0 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-

methoxybenzoyl]amino]-, 1,1-dimethylethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-70-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(3S)-3-pyrrolidinyl- (CA INDEX NAME)

## Absolute stereochemistry.

RN 1201691-71-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(1-piperidinyl)propyl]- (CA INDEX NAME)

RN 1201691-72-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1,2,2,6,6-

pentamethyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201691-73-7 CAPLUS

CN 1-Azetidinecarboxylic acid, 3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201691-74-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(4-methyl-1-piperazinyl)propyl]- (CA INDEX NAME)

RN 1201691-75-9 CAPLUS

CN Benzamide, N-[1-(2-amino-2-methyl-1-oxopropyl)-4-piperidinyl]-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201691-76-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[(4R)-2-oxo-4-piperidinyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-77-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[(4S)-2-oxo-4-

piperidinyl] - (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-78-2 CAPLUS

CN 1-Azetidinecarboxylic acid, 3-[[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201691-80-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(3-pyrrolidinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & MeO & C-NH-CH_2-NH \\ \hline F & N & NH-CH_2-NH \\ \end{array}$$

RN 1201691-82-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(1-piperazinyl)propyl]- (CA INDEX NAME)

RN 1201691-83-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-[4-(2-hydroxyethyl)-1-piperazinyl]propyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-85-1 CAPLUS

CN Benzamide, N-(cis-4-aminocyclohexyl)-4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201691-86-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[(3S)-1-(phenylmethyl)-3-pyrrolidinyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-87-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[(3R)-1-(phenylmethyl)-3-pyrrolidinyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-88-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-4-hydroxy-, 1,1-dimethylethyl ester, (3R,4R)- (CA

INDEX NAME)

Absolute stereochemistry.

RN 1201691-89-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[(3R,4R)-4-hydroxy-3-pyrrolidinyl]-3-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 1201691-90-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(4-hydroxy-1-piperidinyl)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201691-91-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-(2-pyridinyl)-4-piperidinyl]- (CA INDEX NAME)

RN 1201691-92-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(2-pyridinylmethyl)- (CA INDEX NAME)

RN 1201691-93-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(2-methyl-1-piperidinyl)propyl]- (CA INDEX NAME)

Me O Me O C NH- (
$$CH_2$$
) 3 N

RN 1201691-94-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(3-pyridinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & N & MeO & C-NH-CH_2-N \\ \hline F & N & NH-CH_2-N \\ \end{array}$$

RN 1201691-95-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(1-methyl-2-pyrrolidinyl)propyl]- (CA INDEX NAME)

RN 1201691-96-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[3-(2-oxo-1-pyrrolidinyl)propyl]- (CA INDEX NAME)

RN 1201691-97-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)

RN 1201691-98-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(2-pyridinyl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & N & MeO & C-NH-CH_2-CH_2 \\ \hline F & N & NH & NH & NH & NH \\ \end{array}$$

RN 1201691-99-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & MeO & C-NH-CH_2-CH_2-N \end{array}$$

RN 1201692-00-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[2-(phenylamino)ethyl]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ N & C-NH-CH_2-CH_2-NHPh \\ \hline \\ F & N & OMe \\ \end{array}$$

RN 1201692-01-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[3-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201692-02-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-hydroxy-3-(1-piperazinyl)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201692-03-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-[1-(phenylmethyl)-4-piperidinyl]- (CA INDEX NAME)

RN 1201692-04-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(diethylamino)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201692-06-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N,N-dimethyl-(CA INDEX NAME)

RN 1201692-07-0 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro-2-[[2-methoxy-4-(1-piperidinylcarbonyl)phenyl]amino]-5-methyl- (CA INDEX NAME)

RN 1201692-08-1 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro-2-[[2-methoxy-4-(4-morpholinylcarbonyl)phenyl]amino]-5-methyl- (CA INDEX NAME)

RN 1201692-09-2 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro-2-[[2-methoxy-4-[(4-methyl-1-piperazinyl)carbonyl]phenyl]amino]-5-methyl- (CA INDEX NAME)

RN 1201692-10-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-4-pyridinyl-(CA INDEX NAME)

RN 1201692-11-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-3-pyridinyl-(CA INDEX NAME)

RN 1201692-13-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

$$\begin{array}{c|c}
C & \text{NH}_2 \\
\hline
C & \text{NH}_2
\end{array}$$

RN 1201692-14-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-methyl- (CA INDEX NAME)

RN 1201692-15-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & \\ & & \\ & & \\ & \\ & \\ & & \\ & \\ & & \\ & \\ & & \\ & \\ & \\ & & \\ & \\ & \\ & \\ & \\ & \\ &$$

RN 1201692-16-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]- (CA INDEX NAME)

RN 1201692-17-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(tetrahydro-2H-pyran-4-yl)-(CA INDEX NAME)

RN 1201692-18-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-20-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN 1201692-21-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-methyl- (CA INDEX NAME)

RN 1201692-22-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)-(CA INDEX NAME)

RN 1201692-23-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-(CA INDEX NAME)

RN 1201692-24-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(tetrahydro-2H-pyran-4-yl)-(CA INDEX NAME)

RN 1201692-26-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

RN 1201692-27-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-methyl- (CA INDEX NAME)

RN 1201692-28-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-29-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]- (CA INDEX NAME)

RN 1201692-30-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-31-0 CAPLUS

CN Benzamide, 4-[[9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-(2,2,2-trifluoroethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-33-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201692-34-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1201692-35-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201692-36-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-38-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201692-39-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1201692-40-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-41-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{O} \\ | & \text{C-NH-(CH2)}_3 - \text{NMe}_2 \\ \hline \\ F & \text{N} & \text{OMe} \end{array}$$

RN 1201692-42-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-5-ethyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-44-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy- (CA INDEX NAME)

RN 1201692-45-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-methyl-(CA INDEX NAME)

RN 1201692-46-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-47-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ & & & & & & \\ \hline O & & & & & \\ \hline N & & & & \\ \hline F & & & & \\ \hline N & & & & \\ \hline O Me & & & \\ \hline \end{array}$$

RN 1201692-48-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-6-oxo-5-propyl-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-50-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy- (CA INDEX NAME)

RN 1201692-51-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy-N-methyl- (CA INDEX NAME)

RN 1201692-52-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-2-fluoro-5-methoxy- (CA INDEX NAME)

RN 1201692-53-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-54-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-2-fluoro-5-methoxy- (CA INDEX NAME)

RN 1201692-55-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-2-fluoro-5-methoxy- (CA INDEX NAME)

RN 1201692-56-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-(1-methylethoxy)-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-57-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-3-methyl- (CA INDEX NAME)

RN 1201692-58-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methyl-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-59-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-methyl- (CA INDEX NAME)

RN 1201692-60-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \hline \\ \text{O} & \text{NH} \\ \hline \\ \text{F} & \text{N} \\ \end{array}$$

RN 1201692-61-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N,3-dimethyl- (CA INDEX NAME)

RN 1201692-63-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methyl-N-4-piperidinyl-(CA INDEX NAME)

RN 1201692-64-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methyl- (CA INDEX NAME)

RN 1201692-65-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl-N-(1-ethyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-66-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-67-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-ethyl- (CA INDEX NAME)

RN 1201692-68-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-ethyl- (CA INDEX NAME)

RN 1201692-69-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl-N-methyl- (CA INDEX NAME)

RN 1201692-71-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl-N-4-piperidinyl-(CA INDEX NAME)

RN 1201692-72-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethyl- (CA INDEX NAME)

RN 1201692-73-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-74-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(tetrahydro-2H-pyran-4-yl)-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-75-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-76-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-77-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-methyl-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-79-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-4-piperidinyl-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-80-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-(trifluoromethyl)- (CA INDEX NAME)

RN 1201692-81-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy-N-(1-ethyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-82-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-83-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-ethoxy- (CA INDEX NAME)

RN 1201692-84-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-ethoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \hline \\ \text{O} & \text{C-NH-(CH2)}_3 - \text{NMe}_2 \\ \hline \\ \text{F} & \text{N} \\ \end{array}$$

RN 1201692-85-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy-N-methyl- (CA INDEX NAME)

RN 1201692-87-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy-N-4-piperidinyl-(CA INDEX NAME)

RN 1201692-88-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-ethoxy- (CA INDEX NAME)

RN 1201692-89-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-3-fluoro-(CA INDEX NAME)

RN 1201692-90-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluoro-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201692-91-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-3-fluoro-(CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1201692-92-3 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-3-fluoro-(CA INDEX NAME)

Me O 
$$C-NH-(CH_2)_3-NMe_2$$
 F  $R$ 

RN 1201692-93-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluoro-N-methyl- (CA INDEX NAME)

RN 1201692-95-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluoro-N-4-piperidinyl-(CA INDEX NAME)

RN 1201692-96-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-fluoro-(CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1201692-98-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluoro-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201692-99-0 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-2,5-difluoro-(CA INDEX NAME)

RN 1201693-00-6 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluoro-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201693-01-7 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-2,5-difluoro-(CA INDEX NAME)

RN 1201693-02-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-2,5-difluoro-(CA INDEX NAME)

Me 
$$C-NH-(CH_2)_3-NMe_2$$
 $F$ 
 $N$ 
 $N$ 
 $N$ 

RN 1201693-03-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluoro-N-methyl-(CA INDEX NAME)

RN 1201693-05-1 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluoro-N-4-piperidinyl- (CA INDEX NAME)

RN 1201693-06-2 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,5-difluoro- (CA INDEX NAME)

$$\begin{array}{c|c} Me & F & O \\ \hline O & N & NH & F \\ \hline F & N & F \end{array}$$

RN 1201693-07-3 CAPLUS

CN Benzoic acid, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,3-difluoro-, methyl ester (CA INDEX NAME)

RN 1201693-08-4 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,3-difluoro-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201693-09-5 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-2,3-difluoro-(CA INDEX NAME)

RN 1201693-10-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2,3-difluoro-N-methyl-(CA INDEX NAME)

RN 1201693-13-1 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]- (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline O & N \\ \hline F & N \\ \hline \end{array}$$

RN 1201693-14-2 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-methyl- (CA INDEX NAME)

RN 1201693-16-4 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-4-piperidinyl- (CA INDEX NAME)

RN 1201693-17-5 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-ethyl-4-piperidinyl)-(CA INDEX NAME)

RN 1201693-18-6 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(1-methyl-4-piperidinyl)-(CA INDEX NAME)

RN 1201693-19-7 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-

5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-(tetrahydro-2H-pyran-4-yl)-(CA INDEX NAME)

RN 1201693-20-0 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[2-(dimethylamino)ethyl]-(CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O} \\ & \text{O} \\ & \text{N} \\ & \text{$$

RN 1201693-21-1 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[3-(dimethylamino)propyl]-(CA INDEX NAME)

RN 1201693-22-2 CAPLUS

CN Benzamide, 4-[(9-cyclohexyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[1-(2,2-difluoroethyl)-4-piperidinyl]-3-methoxy- (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidodiazepine derivs. for use as PLK1 inhibitors) 1201693-24-4 CAPLUS

Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[2-(2-thienyl)ethyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN

CN

RN 1201693-25-5 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[2-(2-thienyl)ethyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

RN 1201693-26-6 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[2-(2-thienyl)ethyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1201693-27-7 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[2-(2-thienyl)ethyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201693-28-8 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[2-(2-thienyl)ethyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201693-30-2 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenylethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

$$\begin{array}{c|c} Me & & & \\ \hline \\ N & & \\ \hline \\ F & & \\ \hline \\ CH_2-CH_2-Ph \end{array}$$

RN 1201693-31-3 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenylethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

RN 1201693-32-4 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenylethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1201693-33-5 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenylethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

Me O 
$$C-NH-(CH_2)_3-NMe_2$$
 $C-NH-(CH_2)_3-NMe_2$ 
 $CH_2-CH_2-Ph$ 

RN 1201693-34-6 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenylethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201693-36-8 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(3-phenylpropyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201693-37-9 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(3-phenylpropyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

Me O 
$$C-NH_2$$
 $F$ 
 $N$ 
 $N$ 
 $NH$ 
 $OMe$ 
 $OMe$ 

RN 1201693-38-0 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(3-phenylpropyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-methyl- (CA INDEX NAME)

RN 1201693-39-1 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(3-phenylpropyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

Me O 
$$C-NH-(CH_2)_3-NMe_2$$
 $F$  O  $C-NH-(CH_2)_3-NMe_2$ 
 $CH_2)_3-Ph$ 

RN 1201693-40-4 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(3-phenylpropyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

Me MeO C NH 
$$\sim$$
 C NH  $\sim$  C  $\sim$ 

RN 1201693-42-6 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[(1R,2S)-2-phenylcyclopropyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-43-7 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[(1R,2S)-2-phenylcyclopropyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-44-8 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-[(1R,2S)-2-phenylcyclopropyl]-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-N-[3-(dimethylamino)propyl]-3-methoxy-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-45-9 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-9-[(4-methoxyphenyl)methyl]-

5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201693-47-1 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

RN 1201693-48-2 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-methyl-(CA INDEX NAME)

RN 1201693-49-3 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-N-[3-(dimethylamino)propyl]-3-methoxy- (CA INDEX NAME)

RN 1201693-50-6 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(tetrahydro-2H-pyran-4-yl)- (CA INDEX NAME)

RN 1201693-51-7 CAPLUS

CN Benzamide, 4-[(7,7-dichloro-9-cyclopentyl-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201693-52-8 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[cis-4-[4-(cyclopropylmethyl)-1-piperazinyl]cyclohexyl]-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-53-9 CAPLUS

CN Benzamide, 4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-N-[trans-4-[4-(cyclopropylmethyl)-1-piperazinyl]cyclohexyl]-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-54-0 CAPLUS

CN Benzamide, N-[cis-4-[4-(cyclopropylmethyl)-1-piperazinyl]cyclohexyl]-4- [[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-55-1 CAPLUS

CN Benzamide, N-[trans-4-[4-(cyclopropylmethyl)-1-piperazinyl]cyclohexyl]-4[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)-6-oxo-5Hpyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-56-2 CAPLUS

CN Benzamide, 4-[(7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxy-N-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

RN 1201693-57-3 CAPLUS

CN Benzamide, 4-[[7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-9-(2-phenoxyethyl)-5H-pyrimido[4,5-b][1,4]diazepin-2-yl]amino]-3-methoxy-N-(1-

methyl-4-piperidinyl)- (CA INDEX NAME)

ΙT	1062246-01-8P	1062246-03-0P	1137869-50-1P
	1137869-51-2P	1137870-04-2P	1201693-59-5P
	1201693-60-8P	1201693-61-9P	1201693-62-0P
	1201693-63-1P	1201693-64-2P	1201693-65-3P
	1201693-66-4P	1201693-70-0P	1201693-71-1P
	1201693-72-2P	1201693-74-4P	1201693-75-5P
	1201693-77-7P	1201693-78-8P	1201693-80-2P
	1201693-81-3P	1201693-83-5P	1201693-84-6P
	1201693-86-8P	1201693-87-9P	1201693-88-0P
	1201693-90-4P	1201693-91-5P	1201693-94-8P
	1201693-99-3P		

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidodiazepine derivs. for use as PLK1 inhibitors) 1062246-01-8 CAPLUS

RN 1062246-01-8 CAPLUS CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,

2-chloro-9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro- (CA INDEX NAME)

RN 1062246-03-0 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

RN 1137869-50-1 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-9-cyclohexyl-7,7-difluoro-5,7,8,9-tetrahydro- (CA INDEX NAME)

RN 1137869-51-2 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-9-cyclohexyl-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

RN 1137870-04-2 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl-9-(1-methylethyl)- (CA INDEX NAME) 10/560,953

RN 1201693-59-5 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-9-cyclobutyl-7,7-difluoro-5,7,8,9-tetrahydro- (CA INDEX NAME)

RN 1201693-60-8 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-9-cyclobutyl-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

RN 1201693-61-9 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-62-0 CAPLUS

CN Carbamic acid, N-[1-[4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]-4-piperidinyl]-, 9H-fluoren-9-ylmethyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 1201693-63-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]benzoyl]amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-64-2 CAPLUS

CN Carbamic acid, N-[1-[4-[(9-cyclobutyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]benzoyl]-4-piperidinyl]-, 9H-fluoren-9-ylmethyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN

1201693-65-3 CAPLUS Carbamic acid, N-[2-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-CN methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-66-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[[4-[(9-cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-3-methoxybenzoyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 1201693-70-0 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-9-cyclopentyl-5-ethyl-7,7-difluoro-5,7,8,9-tetrahydro- (CA INDEX NAME)

RN 1201693-71-1 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro-5-propyl- (CA INDEX NAME)

RN 1201693-72-2 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-9-cyclopentyl-7,7-difluoro-5,7,8,9-tetrahydro-5-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 1201693-74-4 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-9-[2-(2-thienyl)ethyl]- (CA INDEX NAME)

RN 1201693-75-5 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl-9-[2-(2-thienyl)ethyl]-(CA INDEX NAME)

RN 1201693-77-7 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-9-(2-phenylethyl)- (CA INDEX NAME)

$$\begin{array}{c|c}
C & H & N & N \\
F & N & C1 \\
CH_2-CH_2-Ph
\end{array}$$

RN 1201693-78-8 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl-9-(2-phenylethyl)- (CA INDEX NAME)

Me N N C1 
$$CH_2-CH_2-Ph$$

RN 1201693-80-2 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,

2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-9-(3-phenylpropyl)- (CA INDEX NAME)

RN 1201693-81-3 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl-9-(3-phenylpropyl)- (CA INDEX NAME)

RN 1201693-83-5 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-9-[(1R,2S)-2-phenylcyclopropyl]-,
 rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-84-6 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl-9-[(1R,2S)-2-phenylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 1201693-86-8 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-9-[(4-methoxyphenyl)methyl]- (CA
INDEX NAME)

RN 1201693-87-9 CAPLUS
CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one,
2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-9-[(4-methoxyphenyl)methyl]-5methyl- (CA INDEX NAME)

RN 1201693-88-0 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

RN 1201693-90-4 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2,7,7-trichloro-9-cyclopentyl-5,7,8,9-tetrahydro- (CA INDEX NAME)

RN 1201693-91-5 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2,7,7-trichloro-9-cyclopentyl-5,7,8,9-tetrahydro-5-methyl- (CA INDEX NAME)

RN 1201693-94-8 CAPLUS

CN 6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 2-chloro-7,7-difluoro-5,7,8,9-tetrahydro-5-methyl-9-(2-phenoxyethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & & \\ \hline \text{N} & & \\ \hline \text{F} & & \text{N} & \\ \hline \text{C1} & & \\ \hline \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OPh} \end{array}$$

RN 1201693-99-3 CAPLUS

CN Propanoic acid, 2,2-difluoro-3-[(2-phenylethyl)amino]-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ || \\ \text{EtO-C-CF}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-Ph} \end{array}$$

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:490777 CAPLUS

DOCUMENT NUMBER: 150:472578

TITLE: Preparation of deuterated 3-benzazepine (lorcaserin)

derivatives as 5HT2C modulators

INVENTOR(S): Liu, Julie F.

PATENT ASSIGNEE(S): Concert Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 43pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE		APPLICATION NO.						DATE					
WO	WO 2009051747			A1 20090423		WO 2008-US11804						20081015					
	W:	ΑE,	AG,	AL,	AM,	ΑO,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,
		CA,	CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,
		FI,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,
		KG,	KM,	KN,	KP,	KR,	ΚZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,
		ME,	MG,	MK,	MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,
		PL,	PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	ST,	SV,	SY,	ΤJ,
		TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW		
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HR,	HU,
		ΙE,	IS,	IT,	LT,	LU,	LV,	MC,	MT,	ΝL,	NO,	PL,	PT,	RO,	SE,	SI,	SK,
		TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,
		TG,	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,
		AM,	ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM							
US 20090143363 A1 20090604 US 2008-288013 2008								0081	015								
PRIORITY APPLN. INFO.: US 2007-998960P P 20071015								015									
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): MARPAT 150:472578 GI																	
GI																	

AB Title compds. I [A = ring containing 0-7 D atoms and R = Me, CH2D, CD2H, or CD3, with the provision that when R = Me, ring A contains 1-7 D atoms], and their pharmaceutically acceptable salts, are prepared and disclosed as modulators of 5HT2C receptors. For example, compound II was prepared via Friedel-Crafts alkylation of 2-chloro-2-d1-N-(2-(4-chlorophenyl)ethyl)propanamide (preparation given) to yield racemic II which was resolved into its (R) enantiomer by reaction with L-(+)-tartaric acid. Bioassays for evaluation of metabolic stability were performed (no data given). The invention is also directed to using I to treat an array of diseases including obesity.

IT 1146440-05-2P 1146440-08-5P 1146440-12-1P 1146440-13-2P 1146440-18-7P 1146440-21-2P 1146440-23-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of deuterated benzazepine derivs. as 5HT2C modulators) 1146440-05-2 CAPLUS

CN 1H-3-Benzazepine-1-d, 8-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN

RN 1146440-08-5 CAPLUS

CN 1H-3-Benzazepine-1-d, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-12-1 CAPLUS

CN 1H-3-Benzazepine-1-d, 8-chloro-2,3,4,5-tetrahydro-1-(methyl-d3)- (CA INDEX NAME)

RN 1146440-13-2 CAPLUS

CN 1H-3-Benzazepine-1-d, 8-chloro-2,3,4,5-tetrahydro-1-(methy1-d3)-, (1R)-(CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-18-7 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-(methyl-d3)- (CA INDEX NAME)

RN 1146440-21-2 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-(methyl-d3)-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-23-4 CAPLUS

CN 1H-3-Benzazepine-1,1,5-d3, 7-chloro-2,3,4,5-tetrahydro-5-(methyl-d3)- (CA INDEX NAME)

RN 1146440-24-5 CAPLUS CN 1H-3-Benzazepine-1,1,5-d3, 7-chloro-2,3,4,5-tetrahydro-5-(methyl-d3)-, (5R)- (CA INDEX NAME)

# Absolute stereochemistry.

IT 1146440-16-5P 1146440-22-3P 1146440-26-7P
 1146440-27-8P 1146440-28-9P 1146440-31-4P
 1146440-33-6P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of deuterated benzazepine derivs. as 5HT2C modulators) 1146440-16-5 CAPLUS

CN 1H-3-Benzazepine-1-d, 8-chloro-2,3,4,5-tetrahydro-1-(methyl-d3)-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

#### Absolute stereochemistry.

RN

#### ● HCl

RN 1146440-22-3 CAPLUS CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-(methyl-d3)-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

### 10/560,953

Absolute stereochemistry.

#### ● HCl

RN 1146440-26-7 CAPLUS CN 1H-3-Benzazepine-1,1,2,4,5-d5, 7-chloro-2,3,4,5-tetrahydro-2,4-d2-5-(methyl-d3)-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-27-8 CAPLUS CN 1H-3-Benzazepine-1,1,2,4,5-d5, 7-chloro-2,3,4,5-tetrahydro-2,4-d2-5-methyl-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-28-9 CAPLUS CN 1H-3-Benzazepine-1,1,5-d3, 7-chloro-2,3,4,5-tetrahydro-5-methyl-, (5R)-(CA INDEX NAME)

RN 1146440-31-4 CAPLUS CN 1H-3-Benzazepine-2,4-d2, 8-chloro-2,3,4,5-tetrahydro-2,4-d2-1-(methyl-d3)-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-33-6 CAPLUS CN 1H-3-Benzazepine-2,4-d2, 8-chloro-2,3,4,5-tetrahydro-2,4-d2-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

### 10/560,953

CMF C11 H10 C1 D4 N

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 1146440-57-4 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2, 3, 4, 5-tetrahydro-1-(methyl-d3)-, (1R)-, (2R,3R)-2, 3-dihydroxybutanedioate (2:1) (CA INDEX NAME)

CM 1

CRN 1146440-21-2 CMF C11 H11 C1 D3 N

Absolute stereochemistry.

$$R$$
  $C1$   $CD_3$ 

CM 2

CRN 87-69-4 CMF C4 H6 O6

RN 1146440-65-4 CAPLUS

CN 1H-3-Benzazepine-1,1,5-d3, 7-chloro-2,3,4,5-tetrahydro-5-(methyl-d3)-, (5R)-, (2R,3R)-2,3-dihydroxybutanedioate (2:1) (CA INDEX NAME)

CM 1

CRN 1146440-24-5 CMF C11 H8 C1 D6 N

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 1146440-68-7 CAPLUS

CN 1H-3-Benzazepine-1-d, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)-, (2R,3R)-2,3-dihydroxybutanedioate (2:1) (CA INDEX NAME)

CM 1

CRN 1146440-08-5 CMF C11 H13 C1 D N

10/560,953

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

IT 1146440-41-6P 1146440-47-2P 1146440-56-3P 1146440-64-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of deuterated benzazepine derivs. as 5HT2C modulators)

RN 1146440-41-6 CAPLUS

CN Benzeneethanamine, 4-chloro-N-(2-chloropropyl-2-d)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & & D \\ & & \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH}\text{--}\text{CH}_2\text{--}\text{C}\text{--}\text{Me} \\ & & \\ & & \\ & & \\ \end{array}$$

● HCl

RN 1146440-47-2 CAPLUS

CN Benzeneethanamine, 4-chloro-N-(2-chloropropyl-2,3,3,3-d4)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 1146440-56-3 CAPLUS

CN Benzeneethanamine, 4-chloro-N-(2-chloropropyl-3,3,3-d3)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ | \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH--}\text{CH}_2\text{--}\text{CH--}\text{CD}_3 \\ \end{array}$$

● HCl

RN 1146440-64-3 CAPLUS

CN Benzeneethan- $\beta$ ,  $\beta$ -d2-amine, 4-chloro-N-(2-chloropropyl-2,3,3,3-d4)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

- IT 1146440-10-9P 1146440-20-1P 1146440-25-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of deuterated benzazepine derivs. as 5HT2C modulators) RN 1146440-10-9 CAPLUS
- CN Ethanone, 1-[(1R)-8-chloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl-1-d]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-20-1 CAPLUS

CN Ethanone, 1-[(1R)-8-chloro-1,2,4,5-tetrahydro-1-(methyl-d3)-3H-3-benzazepin-3-yl]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

RN 1146440-25-6 CAPLUS

CN Ethanone, 1-[(1R)-8-chloro-1,2,4,5-tetrahydro-5-d-1-(methyl-d3)-3H-3-benzazepin-3-yl-1,5-d2]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L19 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
                           2008:703346 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                            149:32211
TITLE:
                            Processes for preparing
                            (R)-8-chloro-1-methyl-2, 3, 4, 5-tetrahydro-1h-3-
                            benzazepine intermediates toward serotonin-2C (5-HT2C)
                            receptor agonists
                            Gharbaoui, Tawfik; Tandel, Sagun K.; Ma, You-An;
INVENTOR(S):
                            Carlos, Marlon; Fritch, John Robert
PATENT ASSIGNEE(S):
                            Arena Pharmaceuticals, Inc., USA
SOURCE:
                            PCT Int. Appl., 40 pp.
                            CODEN: PIXXD2
DOCUMENT TYPE:
                            Patent
                            English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                                                APPLICATION NO.
                           KIND
                                   DATE
                                                                           DATE
                           ____
                                   _____
                                                 _____
                                                                           _____
                                                WO 2007-US24900
     WO 2008070111
                            A2
                                    20080612
                                                                           20071204
     WO 2008070111
                            А3
                                   20080807
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
              PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
          TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
              IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
              BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
              GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
              BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
     CA 2670285
                            Α1
                                   20080612
                                                 CA 2007-2670285
                                                                           20071204
                                                 EP 2007-867623
     EP 2099743
                             A2
                                    20090916
                                                                           20071204
             AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
              IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR,
              AL, BA, HR, MK, RS
     JP 2010511711
                            Τ
                                    20100415
                                                 JP 2009-540272
                                                                           20071204
     IN 2009KN01898
                            Α
                                    20090612
                                                 IN 2009-KN1898
                                                                           20090521
     CN 101547892
                            Α
                                   20090930
                                                 CN 2007-80045133
                                                                           20090605
                                                                       P 20061205
PRIORITY APPLN. INFO.:
                                                 US 2006-873036P
                                                                       W 20071204
                                                 WO 2007-US24900
                          CASREACT 149:32211; MARPAT 149:32211
OTHER SOURCE(S):
     Processes for the preparation of (R)-8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-
AB
     benzazepines and their intermediates is presented. Compds. of the present
     invention are useful as serotonin-2C (5-HT2C) receptor agonists for the
     treatment of obesity.
     616201-80-0P
                        847063-13-2P
                                            953789-37-2P
     1030624-41-9P
                         1030624-49-7P
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
         (processes for preparing (R)-8-chloro-1-methyl-2,3,4,5-tetrahydro-1h-3-
         benzazepine intermediates toward serotonin-2C (5-HT2C) receptor
         agonists)
RN
     616201-80-0 CAPLUS
     1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)
CN
```

10/560,953

RN 847063-13-2 CAPLUS

CN 2-Propanol, 1-[[2-(4-chlorophenyl)ethyl]amino]- (CA INDEX NAME)

RN 953789-37-2 CAPLUS

CN Benzeneethanamine, 4-chloro-N-(2-chloropropyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 1030624-41-9 CAPLUS

CN 2-Propanol, 1-[[2-(4-chlorophenyl)ethyl]amino]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 1030624-49-7 CAPLUS CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrate (2:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

## ●1/2 H<sub>2</sub>O

ΙT 616202-92-7P 824430-78-6P 846589-98-8P, (R)-8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine hydrochloride 856681-05-5P 1030624-46-4P RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (processes for preparing (R)-8-chloro-1-methyl-2,3,4,5-tetrahydro-1h-3benzazepine intermediates toward serotonin-2C (5-HT2C) receptor agonists) RN 616202-92-7 CAPLUS 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX CN NAME)

Absolute stereochemistry.

RN 824430-78-6 CAPLUS
CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 616202-92-7

Absolute stereochemistry.

CMF C11 H14 C1 N

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 846589-98-8 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 856681-05-5 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride, hydrate (2:2:1), (1R)- (CA INDEX NAME)

10/560,953

● HCl

●1/2 H<sub>2</sub>O

RN 1030624-46-4 CAPLUS CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)-, (2R,3R)-2,3-dihydroxybutanedioate (1:?) (CA INDEX NAME)

CM 1

CRN 616202-92-7 CMF C11 H14 C1 N

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

L19 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:1474771 CAPLUS

DOCUMENT NUMBER: 148:239014

TITLE: Discovery and Structure-Activity Relationship of

(1R) -8-Chloro-2, 3, 4, 5-tetrahydro-1-methyl-1H-3-

benzazepine (Lorcaserin), a Selective Serotonin 5-HT2C

Receptor Agonist for the Treatment of Obesity

AUTHOR(S): Smith, Brian M.; Smith, Jeffrey M.; Tsai, James H.;

Schultz, Jeffrey A.; Gilson, Charles A.; Estrada, Scott A.; Chen, Rita R.; Park, Douglas M.; Prieto,

Emily B.; Gallardo, Charlemagne S.; Sengupta,

Dipanjan; Dosa, Peter I.; Covel, Jon A.; Ren, Albert; Webb, Robert R.; Beeley, Nigel R. A.; Martin, Michael; Morgan, Michael; Espitia, Stephen; Saldana, Hazel R.;

Bjenning, Christina; Whelan, Kevin T.; Grottick, Andrew J.; Menzaghi, Frederique; Thomsen, William J.

CORPORATE SOURCE: Arena Pharmaceuticals Inc., San Diego, CA, 92121, USA SOURCE: Journal of Medicinal Chemistry (2008), 51(2), 305-313

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:239014

AB The synthesis and SAR of a novel 3-benzazepine series of 5-HT2C agonists is described. Lorcaserin (APD356) was identified as one of the more potent and selective compds. in vitro (pEC50 values in functional assays measuring [3H]phosphoinositol turnover:  $5\text{-HT2C}=8.1;\ 5\text{-HT2A}=6.8;\ 5\text{-HT2B}=6.1)$  and was potent in an acute in vivo rat food intake model upon oral administration (ED50 at 6 h = 18 mg/kg). Lorcaserin was further characterized in a single-dose pharmacokinetic study in rat (t1/2 = 3.7 h; F = 86%) and a 28-day model of weight gain in growing Sprague-Dawley rat (8.5% decrease in weight gain observed at 36 mg/kg b.i.d.). Lorcaserin was selected for further evaluation in clin. trials for the treatment of obesity.

IT 616202-92-7P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship of (1R)-8-chloro-2,3,4,5-tetrahydro-1-methyl-1H-3-benzazepine (Lorcaserin), a selective serotonin 5-HT2C receptor agonist for the treatment of obesity)

RN 616202-92-7 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

(CA INDEX NAME)

RN 616202-87-0 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-7-methoxy-1-methyl-, (1R)-(CA INDEX NAME)

Absolute stereochemistry.

IT 616201-56-0P 616202-81-4P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship of (1R)-8-chloro-2,3,4,5-tetrahydro-1-methyl-1H-3-benzazepine (Lorcaserin), a selective serotonin 5-HT2C receptor agonist for the treatment of obesity)

RN 616201-56-0 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-7-methoxy-1-methyl- (CA INDEX NAME)

RN 616202-81-4 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 23266-24-2 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 25174-38-3 CAPLUS

CN 1H-3-Benzazepine, 7-chloro-2,3,4,5-tetrahydro- (CA INDEX NAME)

RN 616201-80-0 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 616201-86-6 CAPLUS

CN 1H-3-Benzazepine, 8-bromo-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 616201-87-7 CAPLUS

CN 1H-3-Benzazepine, 8-fluoro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 616201-89-9 CAPLUS

CN 1H-3-Benzazepine, 7-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 616201-90-2 CAPLUS

CN 1H-3-Benzazepine, 7,8-dichloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 616202-05-2 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(trifluoromethyl)- (CA INDEX NAME)

RN 616202-08-5 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-7-fluoro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 616202-84-7 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(trifluoromethyl)-, (1S)-(CA INDEX NAME)

Absolute stereochemistry.

RN 616202-85-8 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-1-ethyl-2,3,4,5-tetrahydro-, (1S)- (CA INDEX

NAME)

Absolute stereochemistry.

RN 616202-95-0 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(trifluoromethyl)-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 616202-96-1 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-1-ethyl-2,3,4,5-tetrahydro-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 824430-66-2 CAPLUS

CN 1H-3-Benzazepine, 6,8-dichloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 824430-68-4 CAPLUS

CN 1H-3-Benzazepine, 6-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 824430-69-5 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-9-fluoro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 824430-71-9 CAPLUS

CN 1H-3-Benzazepine, 8,9-dichloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 824430-72-0 CAPLUS

CN 1H-3-Benzazepine, 8,9-dichloro-2,3,4,5-tetrahydro-1-methyl-, (1S)- (CA INDEX NAME)

RN 824430-74-2 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-9-fluoro-2,3,4,5-tetrahydro-1-methyl-, (1S)-(CA INDEX NAME)

Absolute stereochemistry.

RN 824430-76-4 CAPLUS

CN 1H-3-Benzazepine, 8,9-dichloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 849663-02-1 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-7-methoxy-1-methyl- (CA INDEX NAME)

RN 849663-03-2 CAPLUS

CN 1H-3-Benzazepine, 9-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 849663-07-6 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-8-methoxy-1-methyl- (CA INDEX NAME)

RN 1006037-48-4 CAPLUS

CN 1H-3-Benzazepine, 7,8-dichloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1006037-49-5 CAPLUS

CN 1H-3-Benzazepine, 7,8-dichloro-2,3,4,5-tetrahydro-1-methyl-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1006037-50-8 CAPLUS

CN 1H-3-Benzazepine, 7-chloro-2,3,4,5-tetrahydro-8-methoxy-1-methyl- (CA INDEX NAME)

RN 1006037-51-9 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1,1-dimethyl- (CA INDEX NAME)

IT 856681-05-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and structure-activity relationship of (1R)-8-chloro-2,3,4,5-tetrahydro-1-methyl-1H-3-benzazepine (Lorcaserin), a selective serotonin 5-HT2C receptor agonist for the treatment of obesity)

RN 856681-05-5 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride, hydrate (2:2:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

# ●1/2 H<sub>2</sub>O

ΙT	616202-07-4P	616202-11-0P	616202-50-7P
	616202-51-8P	616202-68-7P	616202-78-9P
	616202-80-3P	616202-89-2P	616202-91-6P
	1006037-52-0P	1006037-53-1P	1006037-54-2P

RN

1006037-58-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship of

(1R)-8-chloro-2,3,4,5-tetrahydro-1-methyl-1H-3-benzazepine

(Lorcaserin), a selective serotonin 5-HT2C receptor agonist for the treatment of obesity)

616202-07-4 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-1-ethyl-2,3,4,5-tetrahydro- (CA INDEX NAME)

RN 616202-11-0 CAPLUS

CN Ethanone, 2,2,2-trifluoro-1-(1,2,4,5-tetrahydro-7-methoxy-1-methyl-3H-3-benzazepin-3-yl)- (CA INDEX NAME)

RN 616202-50-7 CAPLUS

CN Ethanone, 1-(8-chloro-1,2,4,5-tetrahydro-1-methylene-3H-3-benzazepin-3-yl)-2,2,2-trifluoro- (CA INDEX NAME)

RN 616202-51-8 CAPLUS

CN Ethanone, 1-(8-chloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl)-2,2,2-trifluoro- (CA INDEX NAME)

RN 616202-68-7 CAPLUS

CN Ethanone, 1-(8-chloro-7-fluoro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl)-2,2,2-trifluoro- (CA INDEX NAME)

RN 616202-78-9 CAPLUS

CN Ethanone, 1-[(1S)-8-chloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

RN 616202-80-3 CAPLUS

CN Ethanone, 1-[(1S)-8-chloro-1-ethyl-1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl]-2,2,2-trifluoro- (CA INDEX NAME)

RN 616202-89-2 CAPLUS

CN Ethanone, 1-[(1R)-8-chloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

RN 616202-91-6 CAPLUS

CN Ethanone, 1-[(1R)-8-chloro-1-ethyl-1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

RN 1006037-52-0 CAPLUS

CN Ethanone, 2,2,2-trifluoro-1-[1,2,4,5-tetrahydro-1-methyl-8-(trifluoromethyl)-3H-3-benzazepin-3-yl]- (CA INDEX NAME)

RN 1006037-53-1 CAPLUS

CN Ethanone, 1-(7,8-dichloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-y1)-2,2,2-trifluoro- (CA INDEX NAME)

RN 1006037-54-2 CAPLUS

CN Benzeneethanamine, 2,3-dichloro-N-(2-chloropropy1)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{C1} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH}\text{--}\text{CH}_2\text{--}\text{CH}\text{--}\text{Me} \end{array}$$

RN 1006037-58-6 CAPLUS

CN Ethanone, 1-(8-chloro-1,2,4,5-tetrahydro-1,1-dimethyl-3H-3-benzazepin-3-yl)-2,2,2-trifluoro- (CA INDEX NAME)

IT 846589-98-8P, Lorcaserin hydrochloride 1006037-59-7P

1006037-60-0P 1006037-61-1P 1006037-62-2P

1006037-63-3P 1006037-65-5P 1006037-66-6P

1006037-67-7P 1006037-69-9P 1006037-71-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and structure-activity relationship of (1R)-8-chloro-2,3,4,5-tetrahydro-1-methyl-1H-3-benzazepine

(Lorcaserin), a selective serotonin 5-HT2C receptor agonist for the

treatment of obesity)

RN 846589-98-8 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

● HCl

RN 1006037-59-7 CAPLUS
CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

HC1

Absolute stereochemistry.

● HCl

RN 1006037-61-1 CAPLUS
CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(trifluoromethyl)-,
hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 1006037-62-2 CAPLUS

CN 1H-3-Benzazepine, 7,8-dichloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 1006037-63-3 CAPLUS

CN 1H-3-Benzazepine, 7,8-dichloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 1006037-65-5 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-7-methoxy-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 1006037-66-6 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-7-methoxy-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 1006037-67-7 CAPLUS

CN 1H-3-Benzazepine, 8,9-dichloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

● HCl

RN 1006037-69-9 CAPLUS
CN 1H-3-Benzazepine, 8,9-dichloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 1006037-71-3 CAPLUS
CN 1H-3-Benzazepine, 8-chloro-9-fluoro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

OS.CITING	REF COUNT:	21	THERE ARE 21 CAPLUS RECORDS THAT CITE THIS
			RECORD (21 CITINGS)
REFERENCE	COUNT:	22	THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
			RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:1204827 CAPLUS

DOCUMENT NUMBER: 147:486344

TITLE: Processes for preparation of

8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine

and intermediates

INVENTOR(S): Weigl, Ulrich; Porstmann, Frank; Straessler,

Christoph; Ulmer, Lars; Koetz, Ulf Arena Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT ASSIGNEE(S):

P	PATENT NO.							KIND DATE			APPL	ICAT		DATE						
		2007120517 0 2007120517									WO 2	007-		20070402						
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,		
			CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,		
			GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,		
			KN,	KP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	MG,	MK,		
			MN,	MW,	MX,	MY,	MZ,	NA,	NG,	ΝI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,		
			RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ΤJ,	TM,	TN,	TR,	TT,		
			TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	ZA,	ZM,	ZW								
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,		
			IS,	IT,	LT,	LU,	LV,	MC,	MT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,		
			ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,		
			GH,	GM,	ΚE,	LS,	MW,	MΖ,	ΝA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,		
			BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	AP,	EA,	EP,	OA							
С	Ά	2646	044			A1		2007	1025		CA 2	007-		20070402						
Ε	Ρ	2001	852			A2		2008	1217		EP 2	007-	7546	20070402						
		R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,		
			IS,	ΙT,	LI,	LT,	LU,	LV,	MC,	MT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,		
			AL,	BA,	HR,	MK,	RS													
		2009						2009			JP 2	009-	5042	48		2	0070	402		
I	N	2008	KN03	623		A		2009 2009	0220					20080904						
											-	007-		20080925						
U	IS	2009	0143.	576		A1		2009	0604		US 2009-225966						20090114			
PRIORI	ΤY	APP:	LN.	INFO	.:						US 2	006-	7891	91P						
							WO 2	007-	US81	70		W 2	0070	402						

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): CASREACT 147:486344

AB The present invention provides a process for the preparation of 8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine, salts, hydrates, and crystal forms thereof. For example, 2-(4-chlorophenyl)ethanol was brominated with phosphorous tribromide, followed by addition of 1-amino-2-propanol and reaction with thionyl chloride to give 4-chloro-N-(2-chloropropyl)benzeneethanamine hydrochloride. The intermediate obtained in the previous step was reacted with aluminum chloride in 1,2-dichlorobenzene, followed by optical resolution with L-tartaric acid to give (R)-8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine hemitartrate. The compds. are useful serotonin (5-HT) receptor agonists for the treatment of central nervous system disorders, such as obesity.

```
ΤТ
     847063-12-1P
     RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT
     (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of 8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine and
        intermediates)
RN
     847063-12-1 CAPLUS
     1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)-,
CN
     (2R, 3R) -2, 3-dihydroxybutanedioate (2:1) (CA INDEX NAME)
     CM
          1
     CRN 616202-92-7
     CMF C11 H14 C1 N
```

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 847063-13-2 CAPLUS

CN 2-Propanol, 1-[[2-(4-chlorophenyl)ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ \mid \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH--}\text{CH}_2\text{--}\text{CH--}\text{Me} \end{array}$$

RN 953789-37-2 CAPLUS

CN Benzeneethanamine, 4-chloro-N-(2-chloropropyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \mid \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH--}\text{CH}_2\text{--}\text{CH--}\text{Me} \end{array}$$

● HCl

IT 616202-81-4P 616202-92-7P 846589-98-8P

856681-05-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine and intermediates)

RN 616202-81-4 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1S)- (CA INDEX NAME)

RN 616202-92-7 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 846589-98-8 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 856681-05-5 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride, hydrate (2:2:1), (1R)- (CA INDEX NAME)

● HCl

●1/2 H<sub>2</sub>O

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L19 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:564968 CAPLUS

DOCUMENT NUMBER: 147:31141

TITLE: Preparation of bicyclic cinnamides as amyloid- $\beta$ 

production inhibitors

INVENTOR(S): Kimura, Teiji; Kawano, Koki; Doi, Eriko; Kitazawa, Noritaka; Takaishi, Mamoru; Ito, Koichi; Kaneko,

Toshihiko; Sasaki, Takeo; Miyagawa, Takehiko;

Hagiwara, Hiroaki; Yoshida, Yu

PATENT ASSIGNEE(S): Eisai R&D Management Co., Ltd., Japan

SOURCE: U.S. Pat. Appl. Publ., 148pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PA:	CENT 1	NO.			KIND DATE				APP	LICAT	DATE									
	US	2007	839		A1						2006- 2006-										
				68				2007													
		2629				A1						2006-					0061				
	WO	2007										2006-					0061				
		W:										B, BG,									
			•	•	•	•	•	•	•	•		E, EC,	•	•	•	•	•	•			
												, IN,									
												LU,									
			MN,	MW,	MX,	MY,	MΖ,	NΑ,	NG,	ΝI,	NO	), NZ,	OM,	PG,	PH,	PL,	PT,	RO,			
			RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM	ı, sv,	SY,	ТJ,	TM,	TN,	TR,	ΤT,			
			TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	ZA,	ZM	1, ZW									
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE	E, ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,			
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT	, RO,	SE,	SI,	SK,	TR,	BF,	ΒJ,			
			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML	, MR,	ΝE,	SN,	TD,	TG,	BW,	GH,			
			GM,	ΚE,	LS,	MW,	MΖ,	NA,	SD,	SL,	SZ	, TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,			
			KG,	KZ,	MD,	RU,	ΤJ,	TM													
	EΡ	1953									EP 2006-822806						0061	101			
		R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE	E, ES,	FI,	FR,	GB,	GR,	HU,	ΙE,			
			IS,	IT,	LI,	LT,	LU,	LV,	MC,	NL,	$_{ m PL}$	, PT,	RO,	SE,	SI,	SK,	TR,	AL,			
				HR,											·			·			
	ZA	2008004446				A		2009	1230		ZA	2008-	4446			20061101					
		5791				A1	2007	1226		AR	2006-										
	ΙN	2008	DN 0 4	111		A		2008	0801		IN	2008-	DN41	11		2	0080	514			
	MX	2008 2008 1013	0064	95		A		2008	0528		MX 2008-6495						0080	520			
	CN	1013	1297	2		А		2008	1126		CN 2006-80043648										
	NO	2008	0028	05		А		2008	0820			2008-					0080	619			
	KR	2008	0720	57		А		2008	0805		KR	2008-	7149	92		2	0080	620			
	US	2009	0181	945		A1		2009	0716		US	2009-	4035	65		2	0090	313			
PRIO	RIT	APP	LN.	INFO	. :						JΡ	2005-	3379	63		A 2	0051	124			
					. •							2006-					0060				
											US	2006-	8337	68P		P 2	0060				
												2006-					0061				
												_ 0 0 0		_ 0 , ,			I				

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): MARPAT 147:31141

GΙ

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- Title compds. I [the solid line accompanied by dotted line represents a AB single or a double bond; Ar1 = Ph, pyridinyl (wherein Ph or pyridinyl may be substituted with substituents selected from halo, hydroxy, cyano, etc.); R1, R2 = halo, hydroxy, cyano, etc.; Z1 = methylene, vinylene, oxygen, etc. (wherein methylene or vinylene may be substituted with substituents selected from halo, hydroxy, cyano, etc.); p, q and r = 0-2] or pharmaceutically acceptable salts thereof were prepared For example, iodination of (3S,8aS)-3-(4-chlorophenyl)hexahydroindolizin-5-one, e.g., prepared from (R)-5-oxopyrrolidine-1,2-dicarboxylic acid 1-tert-Bu 2-Et diester in 12 steps, followed by reaction with tri-Et phosphite and treatment with LiOH afforded compound II. In  $A\beta42$  production-inhibition assays, compound II exhibited the IC50 of 55 nM. Compds. I are claimed useful for the treatment of Alzheimer's disease, senile dementia, etc. 937813-83-7P TТ

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses) (preparation of bicyclic cinnamides as amyloid-β production inhibitors) RN 937813-83-7 CAPLUS

CN Pyrido[1,2-a]azepin-6(2H)-one, 4-(4-fluorophenyl)octahydro-7-[[3-methoxy-4-(4-methyl-1H-imidazol-1-yl)phenyl]methylene]-, (4R,7E,10aR)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

IT 937812-27-6P 937812-28-7P
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
 PREP (Preparation); USES (Uses)

(preparation of bicyclic cinnamides as amyloid- $\beta$  production inhibitors) 937812-27-6 CAPLUS

CN Pyrido[1,2-a]azepin-6(2H)-one, 4-(4-fluorophenyl)octahydro-7-[[3-methoxy-4-(4-methyl-1H-imidazol-1-yl)phenyl]methylene]-, (4S,7E,10aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN

Double bond geometry as shown.

RN 937812-28-7 CAPLUS

CN Pyrido[1,2-a]azepin-6(2H)-one, 4-(4-fluorophenyl)octahydro-7-[[3-methoxy-4-(4-methyl-1H-imidazol-1-yl)phenyl]methylene]-, (4R,7E,10aR)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 937813-79-1P 937813-80-4P 937813-81-5P 937813-82-6P 937816-62-1P 937816-63-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bicyclic cinnamides as amyloid-  $\beta$  production inhibitors) RN 937813-79-1 CAPLUS

CN Pyrido[1,2-a]azepin-6(2H)-one, 4-(4-fluorophenyl)-1,3,4,7,8,10a-hexahydro-, (4R,10aS)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937813-80-4 CAPLUS
CN Pyrido[1,2-a]azepin-6(2H)-one, 4-(4-fluorophenyl)octahydro-, (4R,10aR)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937813-81-5 CAPLUS
CN Pyrido[1,2-a]azepin-6(2H)-one, 4-(4-fluorophenyl)octahydro-7-iodo-, (4R,10aS)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937813-82-6 CAPLUS

CN Phosphonic acid, P-[(4R,10aS)-4-(4-fluorophenyl)decahydro-6-oxopyrido[1,2-a]azepin-7-yl]-, diethyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937816-62-1 CAPLUS

CN Propanoic acid, 2-chloro-3-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(3,4,5-trifluorophenyl)ethyl](methoxycarbonyl)amino]-, ethyl ester (CA INDEX NAME)

RN 937816-63-2 CAPLUS

CN Propanoic acid, 3-[[2-amino-2-(3,4,5-trifluorophenyl)ethyl](methoxycarbonyl)amino]-2-chloro-, ethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

L19 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:409482 CAPLUS

DOCUMENT NUMBER: 142:463621

TITLE: Benzazepine derivatives, their preparation and use for

prophylaxis or treatment of 5HT2C receptor-associated

diseases

INVENTOR(S): Smith, Brian; Schultz, Jeffrey; Gilson, Charles, III;

Estrada, Scott

PATENT ASSIGNEE(S): Arena Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.						KIND DATE				ICAT		DATE				
WC	WO 2005042490					A1 20050512			1	WO 2	004-	US34	20041021				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	B₩,	BY,	BZ,	CA,	CH,
		CN,	СО,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	TG													
US	US 20070275949				A1		2007	1129	1	US 2	006-	5731	20060420				
PRIORIT	PRIORITY APPLN. INFO.:							1	US 2	003-	5138		P 20031022				
						1	WO 2	004-	US34	W 20041021							

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): CASREACT 142:463621; MARPAT 142:463621

GΙ

$$\mathbb{R}^{2}$$
 $\mathbb{N}-\mathbb{R}^{1}$ 
 $\mathbb{R}^{4}$ 

C1 
$$\frac{1}{H}$$
  $\frac{H}{N}$   $\frac{Me}{R^5}$   $N-H$   $\frac{111}{N}$ 

AΒ The invention relates to substituted 2,3,4,5-tetrahydro-3-benzazepine derivs. I, that are modulators of the 5HT2C receptor. In compds. I, R1 is H or C1-8 alkyl; R2 is C1-8 alkyl; R3 is H, aryl, arylalkyloxy, arylalkylamino, arylamino, or heteroaryl, where the N is optionally substituted and where the aryl is optionally substituted with up to two substituents selected from C1-8 alkyl, halo, perhaloalkyl, and alkoxy; R4 is H, arylalkyloxy, alkoxy, or aryloxy; provided that at least one of R3 and R4 is other than H, etc. The invention also relates to the preparation of I, pharmaceutical compns. containing I and a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment of disorders involving 5HT2C receptors. N-Protection of 4-chlorophenethylamine as the trifluoroacetamide followed by iodination and N-allylation resulted in the formation of II. II underwent intramol. Heck reaction followed by hydrogenation, separation of enantiomers, and deprotection to give III [R5 = C1; (S)-enantiomer shown], which, upon N-Boc-protection, substitution with benzylamine, and deprotection, produced III (R5 = NHCH2Ph) as the hydrochloride. Several compds. were tested for 5HT2C agonist activity, with 12 of those having IC50 values between 1 nM and 1.3  $\mu M$  and several others below 10  $\mu M$ . Some compds. of the invention have 3-10 times greater 5HT2C agonist activity than 5HT2B agonist activity.

851478-28-9P, (S)-7-Benzyloxy-1-methyl-2,3,4,5-tetrahydro-1H-ΙT 851544-34-8P benzo[d]azepine hydrochloride 851544-39-3P 851544-44-0P 851544-41-7P 851544-47-3P 851544-49-5P 851544-51-9P 851544-53-1P, 8-Benzyloxy-1-methyl-2,3,4,5-tetrahydro-1Hbenzo[d]azepine hydrochloride 851544-60-0P, (S)-1-Methyl-8-phenyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine hydrochloride 851544-64-4P, 1-Methyl-7-(1-phenylethoxy)-2,3,4,5-tetrahydro-1Hbenzo[d]azepine hydrochloride 851544-66-6P, 1-Methyl-7-phenethyloxy-2,3,4,5-tetrahydro-1H-benzo[d]azepine hydrochloride 851544-67-7P, 1-Methyl-7-(3-phenylpropoxy)-2,3,4,5-tetrahydro-1H-benzo[d]azepine 851544-68-8P, hydrochloride 8-Benzyloxy-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine

```
851544-73-5P, (R)-1-Methyl-8-phenyl-2,3,4,5-tetrahydro-1H-
                              851544-75-7P,
benzo[d]azepine hydrochloride
7-Methoxy-1-methyl-8-phenyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
               851544-77-9P,
hydrochloride
(S)-8-(2-Fluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride
               851544-78-0P,
(S)-8-(3-Fluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
                851544-79-1P,
hydrochloride
(S)-8-(4-Fluoropheny1)-1-methy1-2,3,4,5-tetrahydro-1H-benzo[d]azepine
               851544-80-4P,
hydrochloride
(S)-8-(2,6-Difluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
               851544-81-5P,
hydrochloride
(R)-8-(3-Fluoropheny1)-1-methy1-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride 851544-82-6P,
(R)-8-(4-Fluoropheny1)-1-methy1-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride 851544-83-7P,
(R)-8-(2,3-Difluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride 851544-84-8P,
(S)-8-(2,5-Difluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride 851544-85-9P,
(R)-1-Methyl-8-pyridin-3-yl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride
              851544-86-0P,
1-Methyl-8-pyridin-2-yl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
hydrochloride 851544-89-3P,
7-Benzyloxy-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
851544-90-6P, 1-Methyl-7-(1-phenylethoxy)-2,3,4,5-tetrahydro-1H-
benzo[d]azepine
                 851544-91-7P,
1-Methyl-7-phenethyloxy-2,3,4,5-tetrahydro-1H-benzo[d]azepine
851544-92-8P, 1-Methyl-7-(3-phenylpropoxy)-2,3,4,5-tetrahydro-1H-
benzo[d]azepine 851544-93-9P,
Benzyl[5-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-yl]amine
851544-94-0P, [5-Methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-
yl](1'-phenylethyl)amine 851544-95-1P,
N-Benzyl-N-methyl[5-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-yl]amine
851544-96-2P, N-[5-Methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-
yl]phenethylamine
                   851544-97-3P,
N-[5-Methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-yl](3-
phenylpropyl)amine
                    851544-98-4P,
N-[5-Methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-yl]phenylamine
851544-99-5P, 1-Methyl-8-phenyl-2,3,4,5-tetrahydro-1H-
benzo[d]azepine
                 851545-00-1P,
7-Methoxy-1-methyl-8-phenyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
851545-01-2P, 8-(2-Fluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-
benzo[d]azepine
                 851545-02-3P,
8-(3-Fluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
851545-03-4P, 8-(4-Fluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-
benzo[d]azepine
                851545-04-5P,
8-(2,6-Difluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
851545-05-6P, 8-(2,3-Difluorophenyl)-1-methyl-2,3,4,5-tetrahydro-
1H-benzo[d]azepine
                     851545-06-7P,
8-(2,5-Difluorophenyl)-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
851545-07-8P, 1-Methyl-8-pyridin-3-yl-2,3,4,5-tetrahydro-1H-
                 851545-08-9P,
benzo[d]azepine
1-Methyl-8-pyridin-2-yl-2,3,4,5-tetrahydro-1H-benzo[d]azepine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
```

(drug candidate; preparation of benzazepine derivs. and use as 5HT2C receptor agonists)

RN 851478-28-9 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(phenylmethoxy)-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 851544-34-8 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(phenylmethyl)-, hydrochloride (1:1), (5S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-39-3 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-N,5-dimethyl-N-(phenylmethyl)-, hydrochloride (1:1), (5S)- (CA INDEX NAME)

● HCl

RN 851544-41-7 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-[(1R)-1-phenylethyl]-, hydrochloride (1:1), (5S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-44-0 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-[(1S)-1-phenylethyl]-, hydrochloride (1:1), (5S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-47-3 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-phenyl-, hydrochloride (1:1), (5S)- (CA INDEX NAME)

● HCl

RN 851544-49-5 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(2-phenylethyl)-, hydrochloride (1:1) (CA INDEX NAME)

HC1

RN 851544-51-9 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(3-phenylpropyl)-, hydrochloride (1:1), (5S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-53-1 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(phenylmethoxy)-, hydrochloride (1:1) (CA INDEX NAME)

HC1

RN 851544-60-0 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-phenyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 851544-64-4 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(1-phenylethoxy)-, hydrochloride (1:1) (CA INDEX NAME)

● HC1

RN 851544-66-6 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(2-phenylethoxy)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851544-67-7 CAPLUS CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(3-phenylpropoxy)-, hydrochloride (1:1) (CA INDEX NAME)

$$O-(CH_2)_3-Ph$$
 $Me$ 

HC1

RN 851544-68-8 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(phenylmethoxy)- (CA INDEX NAME)

$$_{
m HN}$$
 O-CH<sub>2</sub>-Ph

RN 851544-73-5 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-phenyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

● HCl

RN 851544-75-7 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-7-methoxy-1-methyl-8-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 851544-77-9 CAPLUS

CN 1H-3-Benzazepine, 8-(2-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-78-0 CAPLUS

CN 1H-3-Benzazepine, 8-(3-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

● HCl

RN 851544-79-1 CAPLUS
CN 1H-3-Benzazepine, 8-(4-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 851544-80-4 CAPLUS
CN 1H-3-Benzazepine, 8-(2,6-difluoropheny1)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-81-5 CAPLUS
CN 1H-3-Benzazepine, 8-(3-fluoropheny1)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 851544-82-6 CAPLUS
CN 1H-3-Benzazepine, 8-(4-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-83-7 CAPLUS

CN 1H-3-Benzazepine, 8-(2,3-difluorophenyl)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-84-8 CAPLUS
CN 1H-3-Benzazepine, 8-(2,5-difluoropheny1)-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 851544-85-9 CAPLUS
CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(3-pyridinyl)-, hydrochloride (1:?), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

•x HCl

RN 851544-86-0 CAPLUS CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(2-pyridinyl)-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 851544-89-3 CAPLUS CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(phenylmethoxy)- (CA INDEX NAME)

RN 851544-90-6 CAPLUS CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(1-phenylethoxy)- (CA INDEX NAME)

RN 851544-91-7 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(2-phenylethoxy)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{O-CH}_2\text{-CH}_2\text{-Ph} \\ \\ \text{Me} \end{array}$$

RN 851544-92-8 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-7-(3-phenylpropoxy)- (CA INDEX NAME)

RN 851544-93-9 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(phenylmethyl)-(CA INDEX NAME)

RN 851544-94-0 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(1-phenylethyl)-(CA INDEX NAME)

RN 851544-95-1 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-N,5-dimethyl-N-(phenylmethyl)-(CA INDEX NAME)

RN 851544-96-2 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(2-phenylethyl)-(CA INDEX NAME)

RN 851544-97-3 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-(3-phenylpropyl)-(CA INDEX NAME)

RN 851544-98-4 CAPLUS

CN 1H-3-Benzazepin-7-amine, 2,3,4,5-tetrahydro-5-methyl-N-phenyl- (CA INDEX NAME)

RN 851544-99-5 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-phenyl- (CA INDEX NAME)

RN 851545-00-1 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-7-methoxy-1-methyl-8-phenyl- (CA INDEX NAME)

RN 851545-01-2 CAPLUS

CN 1H-3-Benzazepine, 8-(2-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 851545-02-3 CAPLUS

CN 1H-3-Benzazepine, 8-(3-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 851545-03-4 CAPLUS

CN 1H-3-Benzazepine, 8-(4-fluorophenyl)-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 851545-04-5 CAPLUS

CN 1H-3-Benzazepine, 8-(2,6-difluorophenyl)-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 851545-05-6 CAPLUS

CN 1H-3-Benzazepine, 8-(2,3-difluorophenyl)-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 851545-06-7 CAPLUS

CN 1H-3-Benzazepine, 8-(2,5-difluorophenyl)-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN 851545-07-8 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(3-pyridinyl)- (CA INDEX NAME)

RN 851545-08-9 CAPLUS

CN 1H-3-Benzazepine, 2,3,4,5-tetrahydro-1-methyl-8-(2-pyridinyl)- (CA INDEX NAME)

ΙT 616202-50-7P, N-Trifluoroacetyl-8-chloro-1-methylene-2,3,4,5tetrahydro-1H-3-benzazepine 616202-51-8P, N-Trifluoroacety1-8-chloro-1-methy1-2,3,4,5-tetrahydro-1H-3-benzazepine 616202-78-9P, (S)-N-Trifluoroacetyl-8-chloro-1-methyl-2,3,4,5tetrahydro-1H-3-benzazepine 616202-81-4P, (S)-8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine 851477-54-8P, (S)-N-tert-Butoxycarbonyl-8-chloro-1-methyl-2,3,4,5tetrahydro-1H-benzo[d]azepine 851478-25-6P, (S)-N-Trifluoroacetyl-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-7-ol 851478-27-8P, (S)-N-Trifluoroacetyl-7-benzyloxy-1-methyl-2,3,4,5tetrahydro-1H-benzo[d]azepine 851544-37-1P 851544-56-4P, 8-Hydroxy-1-methyl-2-oxo-2,3,5-trihydro-1Hbenzo[d]azepine 851544-58-6P, 8-Benzyloxy-1-methyl-2-oxo-2,3,5-trihydro-1H-benzo[d]azepine 851544-62-2P 851544-69-9P, 1-[[2-(4-Methoxyphenyl)ethyl]amino]propan-2-ol 851544-70-2P, (2-Bromopropyl) [2-(4-methoxyphenyl)ethyl]amine hydrobromide 851544-71-3P, N-tert-Butoxycarbonyl-5-methyl-2,3,4,5-tetrahydro-1Hbenzo[d]azepin-7-ol 851544-72-4P, N-tert-Butoxycarbonyl-8-benzyloxy-1-methyl-2,3,4,5-tetrahydro-1H-

benzo[d]azepine 851544-74-6P, (R)-N-tert-Butoxycarbonyl-1-methyl-8-phenyl-1,2,4,5tetrahydrobenzo[d]azepine 851544-76-8P, N-Trifluoroacetyl-7-Methoxy-1-methyl-8-phenyl-2,3,4,5-tetrahydro-1Hbenzo[d]azepine 851544-87-1P, Trifluoromethanesulfonic acid N-tert-butoxycarbonyl-5-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepin-8-yl 851544-88-2P, N-tert-Butoxycarbonyl-1-methyl-8-pyridin-2y1-2,3,4,5-tetrahydro-1H-benzo[d]azepine RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of benzazepine derivs. and use as 5HT2C receptor agonists) 616202-50-7 CAPLUS RN Ethanone, 1-(8-chloro-1,2,4,5-tetrahydro-1-methylene-3H-3-benzazepin-3-yl)-CN 2,2,2-trifluoro- (CA INDEX NAME)

RN 616202-51-8 CAPLUS CN Ethanone, 1-(8-chloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl)-2,2,2-trifluoro- (CA INDEX NAME)

RN 616202-78-9 CAPLUS
CN Ethanone, 1-[(1S)-8-chloro-1,2,4,5-tetrahydro-1-methyl-3H-3-benzazepin-3-yl]-2,2,2-trifluoro- (CA INDEX NAME)

Absolute stereochemistry.

RN 616202-81-4 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 851477-54-8 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 8-chloro-1,2,4,5-tetrahydro-1-methyl-, 1,1-dimethylethyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 851478-25-6 CAPLUS

CN Ethanone, 2,2,2-trifluoro-1-[(1S)-1,2,4,5-tetrahydro-7-hydroxy-1-methyl-3H-3-benzazepin-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 851478-27-8 CAPLUS

CN Ethanone, 2,2,2-trifluoro-1-[(1S)-1,2,4,5-tetrahydro-1-methyl-7-(phenylmethoxy)-3H-3-benzazepin-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 851544-37-1 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-1-methyl-8-[(phenylmethyl)amino]-, 1,1-dimethylethyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 851544-56-4 CAPLUS

CN 2H-3-Benzazepin-2-one, 1,3,4,5-tetrahydro-8-hydroxy-1-methyl- (CA INDEX NAME)

RN 851544-58-6 CAPLUS

CN 2H-3-Benzazepin-2-one, 1,3,4,5-tetrahydro-1-methyl-8-(phenylmethoxy)- (CA INDEX NAME)

RN 851544-62-2 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-1-methyl-8-phenyl-, 1,1-dimethylethyl ester, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 851544-69-9 CAPLUS

CN 2-Propanol, 1-[[2-(4-methoxyphenyl)ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ \mid \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH}\text{--}\text{CH}_2\text{--}\text{CH}\text{--}\text{Me} \\ \\ \text{MeO} \end{array}$$

RN 851544-70-2 CAPLUS

CN Benzeneethanamine, N-(2-bromopropyl)-4-methoxy-, hydrobromide (1:1) (CA INDEX NAME)

$$\begin{array}{c} \operatorname{Br} \\ \mid \\ \operatorname{CH}_2-\operatorname{CH}_2-\operatorname{NH}-\operatorname{CH}_2-\operatorname{CH}-\operatorname{Me} \end{array}$$

● HBr

RN 851544-71-3 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-8-hydroxy-1-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 851544-72-4 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-1-methyl-8-(phenylmethoxy)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 851544-74-6 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-1-methyl-8-phenyl-, 1,1-dimethylethyl ester, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 851544-76-8 CAPLUS

CN Ethanone, 2,2,2-trifluoro-1-(1,2,4,5-tetrahydro-7-methoxy-1-methyl-8-phenyl-3H-3-benzazepin-3-yl)- (CA INDEX NAME)

RN 851544-87-1 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-1-methyl-7-[[(trifluoromethyl)sulfonyl]oxy]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 851544-88-2 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 1,2,4,5-tetrahydro-1-methyl-8-(2-pyridinyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

IT 616202-92-7 1019636-37-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzazepine derivs. and use as 5HT2C receptor agonists)

RN 616202-92-7 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1019636-37-3 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 8-chloro-1,2,4,5-tetrahydro-1-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

IT 616202-12-1, N-Trifluoroacetyl-8-bromo-7-methoxy-1-methyl-

2,3,4,5-tetrahydro-1H-benzo[d]azepine 851477-82-2,

(R)-N-tert-Butoxycarbonyl-8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine 851478-26-7,

(S)-N-Trifluoroacety1-7-methoxy-1-methy1-2,3,4,5-tetrahydro-1H-benzo[d]azepine

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of benzazepine derivs. and use as 5HT2C receptor agonists)

RN 616202-12-1 CAPLUS

CN Ethanone, 1-(8-bromo-1,2,4,5-tetrahydro-7-methoxy-1-methyl-3H-3-benzazepin-3-yl)-2,2,2-trifluoro- (CA INDEX NAME)

RN 851477-82-2 CAPLUS

CN 3H-3-Benzazepine-3-carboxylic acid, 8-chloro-1,2,4,5-tetrahydro-1-methyl-, 1,1-dimethylethyl ester, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 851478-26-7 CAPLUS

CN Ethanone, 2,2,2-trifluoro-1-[(1S)-1,2,4,5-tetrahydro-7-methoxy-1-methyl-3H-3-benzazepin-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:182631 CAPLUS

DOCUMENT NUMBER: 142:280072

TITLE: Processes for preparing 3-benzazepines

Burbaum, Beverly W.; Gilson, Charles A., III; Aytes, INVENTOR(S): Shelley; Estrada, Scott A.; Sengupta, Dipanjan; Smith,

Brian; Rey, Max; Weigl, Ulrich

Arena Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 143 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PA	PATENT NO.				KIND DATE		APPLICATION NO.					DATE						
WO					A2					WO 2004-US19279								
	W:	CN, GE, LK, NO,	CO, GH, LR, NZ,	CR, GM, LS, OM,	CU, HR, LT, PG,	CZ, HU, LU, PH,	AU, DE, ID, LV, PL,	DK, IL, MA, PT,	DM, IN, MD, RO,	DZ, IS, MG, RU,	EC, JP, MK, SC,	EE, KE, MN, SD,	EG, KG, MW, SE,	ES, KP, MX, SG,	FI, KR, MZ, SK,	GB, KZ, NA, SL,	GD, LC, NI, SY,	
		BW, AZ, EE, SI, SN,	GH, BY, ES, SK, TD,	GM, KG, FI, TR, TG	KE, KZ, FR, BF,	LS MD GB BJ	MW, RU, GR, CF,	MZ, TJ, HU, CG,	NA, TM, IE, CI,	SD, AT, IT, CM,	SL, BE, LU, GA,	SZ, BG, MC, GN,	TZ, CH, NL, GQ,	UG, CY, PL, GW,	ZM, CZ, PT, ML,	ZW, DE, RO, MR,	AM, DK, SE, NE,	
CA	2004: 2529: 1636:	401 191			A1 A2		2005 2006	0303 0322		CA 2 EP 2	004- 004-	2529 8018	401 95		2 2	0040 0040	616 616	
	R:						ES,											מט
BR	1805; 2004; 2007; 1012; 2189;	939 0116	13		A A		2006	0719 0808		CN 2 BR 2	004-	8001 1161	6780 3		2	0040	616 616	пк
MX KR IN TN	R: 2005 2006 2006 2391	AT, IT, 0133 0231 KN00	BE, LI, 64 63 112	BG, LU,	CH, MC, A A A	CY,	CZ, PL, 2006 2006 2007 2010	DE, PT, 0317 0313 0316	DK, RO,	EE, SE, MX 2	ES, SI, 005-	FI, SK, 1336	FR, TR, 4	GB, AL,	GR, HR, 2	HU, LT, 0051	IE, LV, 208	MK
US	2008	0045 KN00	502 311		A1		2008	0221		US 2 IN 2 US 2 US 2 CN 2 EP 2 WO 2	007- 009- 003- 003- 004- 004-	5609 KN31 4792 5129 8001 8018 US19 KN11	53 1 80P 67P 6780 95 279		2 P 2 P 2 A3 2 A3 2	0070 0090 0030 0031 0040 0040	426 121 617 021 616 616	
ASSIGNMI	ENT H	ISTO:	RY F	OR U			ΓAVA		LE I	N LS	US D	ISPL	AY F	ORMA			110	

OTHER SOURCE(S): CASREACT 142:280072; MARPAT 142:280072

GI

$$R^4$$
 $R^3$ 
 $R^2$ 
 $N-R^1$ 
 $R^6$ 
 $R^8$ ?  $R^8$ ?  $R^7$ ?  $R^7$ ?  $R^8$ 

AB A process for the preparation of 3-benzazepines I [R1 = H; R2 = alkyl, alkoxy, carboxy, etc.; R3-6 = H, halo, alk(en/yn)yl, etc.; R7a-7b = H, halo, alk(en/yn)yl, etc.; R8a-8b = H, halo, alk(en/yn)yl, etc.] is disclosed. For instance, 2-(4-chlorophenyl)ethylamine is acylated with 2-chloropropionyl chloride (CH3CN, Et3N). The resulting amide is cyclized in the presence of a metal hydride, e.g., AlCl3 to the corresponding benzazepin-2-one. Reduction of this amide is accomplished with BH3 in THF to give II. Alternative, but similar procedures are provided and there are examples of resolution of the final product by formation of the L-tartaric acid salts. I are useful as serotonin (5-HT) receptor agonists [no data] for the treatment of, e.g., central nervous system disorders such as obesity.

IT 616201-80-0P, 8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(processes for preparing 3-benzazepines as 5-HT receptor agonists) 616201-80-0 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl- (CA INDEX NAME)

RN

IT 846589-98-8P, (R)-8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine hydrochloride

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(processes for preparing 3-benzazepines as  $5-\mathrm{HT}$  receptor agonists) 846589-98-8 CAPLUS

RN 846589-98-8 CAPLUS
CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, hydrochloride (1:1), (1R)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

ΙT 824430-77-5P, 8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3benzazepin-2-one 847063-12-1P 847063-13-2P, 1-[[2-(4-Chlorophenyl)ethyl]amino]-2-hydroxypropane 847063-14-3P , 1-[[2-(4-Chlorophenyl)ethyl]amino]-2-bromopropane 897926-35-1P RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (processes for preparing 3-benzazepines as 5-HT receptor agonists) 824430-77-5 CAPLUS RN 2H-3-Benzazepin-2-one, 8-chloro-1,3,4,5-tetrahydro-1-methyl- (CA INDEX CN NAME)

RN 847063-12-1 CAPLUS
CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)-, (2R,3R)-2,3-dihydroxybutanedioate (2:1) (CA INDEX NAME)

CM 1

CRN 616202-92-7 CMF C11 H14 C1 N

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

847063-13-2 CAPLUS RN

CN 2-Propanol, 1-[[2-(4-chlorophenyl)ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ | \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH}\text{--}\text{CH}_2\text{--}\text{CH}\text{--}\text{Me} \end{array}$$

RN 847063-14-3 CAPLUS

Benzeneethanamine, N-(2-bromopropyl)-4-chloro- (CA INDEX NAME) CN

$$\begin{array}{c} \operatorname{Br} \\ | \\ \operatorname{CH}_2-\operatorname{CH}_2-\operatorname{NH}-\operatorname{CH}_2-\operatorname{CH}-\operatorname{Me} \\ \end{array}$$

RN 897926-35-1 CAPLUS

CN Benzeneethanamine, 4-chloro-N-(2-chloropropy1)- (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \mid \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH--}\text{CH}_2\text{--}\text{CH--}\text{Me} \\ \\ \text{C1} \end{array}$$

616202-92-7, (R)-8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-ΙT benzazepine

RL: RCT (Reactant); RACT (Reactant or reagent) (processes for preparing 3-benzazepines as 5-HT receptor agonists)

RN 616202-92-7 CAPLUS

CN 1H-3-Benzazepine, 8-chloro-2,3,4,5-tetrahydro-1-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD

(3 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1997:722 CAPLUS

DOCUMENT NUMBER: 126:86522

ORIGINAL REFERENCE NO.: 126:16641a, 16644a

TITLE: Synthesis of nonpeptide, protease-binding compounds

and diagnostic or therapeutic uses for detecting or

inhibiting retroviral proteases

INVENTOR(S): Ortiz de Montellano, Paul R.; Kuntz, Irwin D.; Craik,

Charles S.; Furth, Paul S.; Alvarez, Juan C.; Caldera, Patricia S.; Decamp, Dianne L.; Babe, Lilia M.; De

Voss, James; Salto, Rafael; Sui, Zhihua

PATENT ASSIGNEE(S): The Regents of the University of California, USA

SOURCE: U.S., 71 pp., Cont.-in-part of U.S. Ser. No. 753,878,

abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5583000	A	19961210	US 1993-122792	19930916
PRIORITY APPLN. INFO.:			US 1991-753878	B2 19910903
ASSIGNMENT HISTORY FOR U	JS PATENT	r available	IN LSUS DISPLAY FOR	TAMS

OTHER SOURCE(S): MARPAT 126:86522

AB Non-peptide, protease-binding compds. are synthesized and characterized. These compds. are useful in the detection of retroviral proteinase in a biol. sample, inhibiting precursor protein processing by retroviral proteinases in living cells, or labeling retroviral proteinases. Haloperidol derivs. and analogs are indexed, as well as LD50, IC50, therapeutic index, HIV-2 proteinase inhibitory activity, and solubility of the compds. Aryl piperidinyl derivs. and other compds. related in structure bind to HIV-1 and HIV-2 proteases.

IT 185625-85-8P

RL: ARG (Analytical reagent use); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation, inhibitor activity, and use; synthesis of nonpeptide, protease-binding compds. and diagnostic or therapeutic uses for detecting or inhibiting retroviral proteases)

RN 185625-85-8 CAPLUS

CN 4-Piperidinol, 4-(4-chlorophenyl)-1-[3-[3-(4-fluorophenyl)-1,5-dihydro-2,4-benzodithiepin-3-yl]propyl]- (CA INDEX NAME)

C1 
$$(CH_2)_3$$
  $S$   $OH$ 

IT 185626-75-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with chlorophenyl hydroxypiperidine; synthesis of nonpeptide,
protease-binding compds. and diagnostic or therapeutic uses for
detecting or inhibiting retroviral proteases)

RN 185626-75-9 CAPLUS

CN Benzeneethanamine, N-(2-chloropropyl)-N-(phenylmethyl)- (CA INDEX NAME)

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD

(4 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1968:12074 CAPLUS

DOCUMENT NUMBER: 68:12074 ORIGINAL REFERENCE NO.: 68:2271a

TITLE: Chemistry of nitrogen radicals. VI. The free-radical

addition of dialkyl-N-chloramines to substituted

olefins

AUTHOR(S): Neale, Robert S.; Marcus, Nancy L.

CORPORATE SOURCE: Union Carbide Res. Inst., Tarrytown, NY, USA

SOURCE: Journal of Organic Chemistry (1967), 32(11), 3273-84

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 68:12074

AB The facile synthesis of a variety of substituted  $\beta$ -chloramines was accomplished in 46-92% yield by the free-radical addition of N-chlorodialkylamines to vinyl and allyl compds. in H2SO4-HOAc. These 1-step reactions are sufficiently general to constitute the method of choice for the preparation of the novel adducts described. The results are also of mechanistic significance, since they demonstrate further that addition to multiple C-C bonds is a reaction characteristic of aminium radicals generated from chloramines. The results also provide further data pertaining to the steric requirements of the addition reaction with vinyl chlorides and to previously recognized competitive processes involving either aminium radical rearrangement or electrophilic chlorination by the protonated chloramine. 36 references.

IT 13426-41-0P 13426-42-1P 13426-43-2P

13426-66-9P 13444-39-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 13426-41-0 CAPLUS

CN Benzeneethanamine, N-(2,2-dichloropropyl)-N-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ | \\ \text{Ph-CH}_2\text{--}\text{CH}_2\text{--}\text{N-CH}_2\text{--}\text{CCl}_2\text{--}\text{Me} \end{array}$$

RN 13426-42-1 CAPLUS

CN Benzeneethanamine, N-(2,2-dichloropropyl)-N-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 13426-43-2 CAPLUS

CN Benzeneethanamine, N-(2,2-dichloropropy1)-N-methyl-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 13426-41-0 CMF C12 H17 C12 N

 $\begin{array}{c} \text{Me} \\ | \\ \text{Ph-CH}_2\text{--CH}_2\text{--N-CH}_2\text{--CCl}_2\text{--Me} \end{array}$ 

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

O<sub>2</sub>N NO<sub>2</sub> OH NO<sub>2</sub>

RN 13426-66-9 CAPLUS
CN 3-Azabicyclo[3.2.2]nonane, 3-(2,2-dichloropropyl)-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 13444-39-8 CMF C11 H19 C12 N

$$\begin{array}{c} \text{N} \\ \text{CH}_2\text{--}\text{CCl}_2\text{--}\text{Me} \end{array}$$

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

RN 13444-39-8 CAPLUS

CN 3-Azabicyclo[3.2.2]nonane, 3-(2,2-dichloropropyl)- (CA INDEX NAME)

N CH2-CCl2-Me

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD

(1 CITINGS)

L15 ANSWER 25 OF 25 REGISTRY COPYRIGHT 2010 ACS on STN

RN 27487-50-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzeneethanamine, N-(2-chloropropyl)-3,4-dimethoxy-N-methyl-, hydrochloride (1:1) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzeneethanamine, N-(2-chloropropy1)-3,4-dimethoxy-N-methyl-, hydrochloride (9CI)

MF C14 H22 C1 N O2 . C1 H

CRN (46906-45-0)

HCl

L15 ANSWER 20 OF 25 REGISTRY COPYRIGHT 2010 ACS on STN

RN 760140-60-1 REGISTRY

ED Entered STN: 10 Oct 2004

CN Benzeneethanaminium, N-(2,3-dibromo-2-methylpropyl)-N,N-dimethyl- $\beta$ -oxo- (CA INDEX NAME)

MF C14 H20 Br2 N O

CI COM

SR CA

$$\begin{array}{c|cccc} \text{O} & \text{Me} & \text{Br} \\ || & | & | \\ \text{Ph-C-CH}_2 - \text{N} & \text{CH}_2 - \text{C-CH}_2 \text{Br} \\ | & | & | \\ \text{Me} & \text{Me} \end{array}$$

L15 ANSWER 21 OF 25 REGISTRY COPYRIGHT 2010 ACS on STN

RN 736891-83-1 REGISTRY

ED Entered STN: 01 Sep 2004

CN 1-Butene-1, 4-diaminium, 3-bromo-N1, N1, N1, N4, N4, 2-hexamethyl-N4-(2-oxo-2-phenylethyl)- (CA INDEX NAME)

MF C18 H29 Br N2 O

CI COM

SR CA

L15 ANSWER 22 OF 25 REGISTRY COPYRIGHT 2010 ACS on STN

RN 47737-72-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzeneethanaminium, N,N-dimethyl-N-(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)- (CA INDEX NAME)

MF C18 H17 F15 N

CI COM

$$\begin{array}{c} \text{Me} \\ \text{Ph-CH}_2\text{--}\text{CH}_2\text{---}\text{N} \\ \text{----} \\ \text{Me} \end{array}$$

L15 ANSWER 23 OF 25 REGISTRY COPYRIGHT 2010 ACS on STN

RN 46906-45-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzeneethanamine, N-(2-chloropropyl)-3,4-dimethoxy-N-methyl- (CA INDEX

MF C14 H22 C1 N O2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L15 ANSWER 24 OF 25 REGISTRY COPYRIGHT 2010 ACS on STN
RN 27487-51-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzeneethanamine, N-(2-chloropropyl)-3,4-dimethoxy-N-methyl-,
ethanedioate (1:1) (CA INDEX NAME)
MF C14 H22 C1 N O2 . C2 H2 O4

CM 1

CRN 46906-45-0 CMF C14 H22 C1 N O2

CM 2

CRN 144-62-7

CMF C2 H2 O4